CrystalClear

Software User's Guide for the
Rigaku R-AXIS, and
Mercury and Jupiter CCD Automated X-ray Imaging Systems
Version 1.3

MOLECULAR STRUCTURE CORPORATION

a Rigaku *company*

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CrystalClear User's Manual (Abridged)
Or
What To Do After You've Started Your Data Collection

INDEX 1. Use the **reciprocal space lattice spacing ruler** to see what the maximum "cell" length is...use 1.5-2x for max. Remember that this is for the *primitive* cell.

FIND, INDEX, REFINE 2. *Find* and *index* off **one image**, then *find* and *refine* off **several images** throughout phi space.

REFINE 3. Although **refinement** from a single image is okay, sometimes better results can be obtained with one of the following strategies for indexing and refining: two images 90 degrees apart; a 5 to 10 degree wedge of data; 2 or 3 images at three different areas of space

REFINE, INTEGRATION 4. **RMS values** on a few images should be close to zero (values around a few pixels and half the image rotation width are to be expected when the mosaicity is not well known). During integration, 3-dimensional data should lead to better determinations of crystal parameters and the RMS values should drop. The RMS for mm should be about 1/10 to 1/5 the spot width; the RMS on phi depends on the image width and mosaicity, in general being between 1/2 the image width and 1/2 the true mosaicity. With 3-dimensional data, RMS degree should be 1/10 to 1/5 the spot size in phi.

REFINE 5. If the refinement **does not use most of the spots** found in the Find step, it is usually because too many peaks are excluded (the resolution limits are too restrictive or the sigma cutoff is too high); rejecting criteria are too strict (x and y max difference too low, phi too small); or there is an incorrect unit cell. Split crystals should have rejected spots not matching the predicted positions. Prediction of spot positions should confirm or deny the choice of unit cell.

REFINE, INTEGRATION 6. By default, any parameters turned on during **refinement** at the refine step will be used in the refinement during integration. It is possible, and likely, that the

mosaicity is turned on during the refinement of the cell after indexing, but it is not refined--this is because you may not have enough rocking curves determined from contiguous images to do a proper calculation of the mosaicity (not necessary, but may be conducted at this step).
INTEGRATION 7. Look in the find log file for the average peaks size and calculate 6 to 10 times this size as a good starting **integration box size**. Then confirm that there is not any critical overlap of adjacent spots using a test prediction and changing the size of the circle. By increasing/decreasing the circle size using the set reflection size button, see that a circle includes no more than half of an adjacent reflection (maximum size). The minimum size of the box cannot be smaller than including all of the area of the peak and considering all regions of the image (although setting it this small is not recommended).
INTEGRATION 8. Images per **batch** is the number of images used in obtaining a refinement and scaling "batch" of reflections--10 or more is typical for small molecule data sets, while 2 to 4 may be used for macromolecular crystals. This is to allow for enough reflections to be available for proper treatment of refinement and scaling...too few will result in poor refinement or refinement crashing, too many will increase memory use beyond installed resources (causing swapping and slowing the calculation).
INTEGRATION 9. **Padding** is the number of images before and after the extent of the reflection (including calculated center and mosaicity) in which some of the background of a particular reflection is determined. In wide slice data, a value of zero may be

particular reflection is determined. In wide slice data, a value of zero may be appropriate, otherwise values of one or two are typical.
INTEGRATION 10. At the start of integration, always have the **processing updates** turned on and carefully observe the agreement between the predicted and observed spot positions.
INTEGRATION 11. During integration, **refinement shifts** for each parameter should be zero. Otherwise you may have crystal movement (sliding, precession, mount instability, etc), too small a batch, or a wrong cell refinement altogether.
INTEGRATION 12. Check to see that the profile fitting correlations are good in the integration log file...both in number and in intensity. Reflections of 9 sigma and higher should have greater than 90% correlation, but may show lower correlation!
SCALING 13. When scaling the data, **absorption correction** should be run in the every attempt. The new algorithm needs fresh information from the absorption calculation. The calculation is relatively fast.
SCALING 14. A good subsequent approximation for the **Weight Addend** is the Rmerge of your current result. Consider using Auto-Rmerge.
SCALING 15. A good subsequent approximation for the **Weight Multiplier** is the square root of the Chi Square multiplied by the current Weight Multiplier. Consider using Auto-Intelligent.

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ASSIGN UNIT CELL:

1. FINDS SPOTS – Select the images on which you want to find spots. Adjust sigma higher or lower depending on the crystal. Typically the 4 screen images are enough to get a good unit cell, again adjust the number of images based on the crystal. For poorly diffracting crystals it is not unusual to find on all images of the first scan. ADVANCED – Lower peak filter to increase the number of spots found. Increase the filter to find any large size spots. The box size can be set to 0 x 0, if necessary, which lets the program pick the best box size, so do not be afraid to try this and work from there.
2. INDEX – You should always check the USER CHOOSES SOLUTION. This allows you to choose an appropriate Laue group.

ADVANCED – Gives some brute force options. Most are self-explanatory. Setting the Max-Residual to 100 will cause indexing to show all Laue classes. 1D-FFT, without difference vectors is currently the preferred method for unit-cell determination.

3. REFINE – A typical starting point is "All", which refines all parameters except the wavelength and is currently the best option. Resolution can be set here if you wish, this can be used to eliminate outliers at high resolution, etc. I/σ can be set to the value you used to find spots. RMS Residuals should be low (ie. Less than 0.5 mm and 0.3 degrees). You want to have most of your reflections accepted. Not using a large percentage of your reflections may indicate problems with the unit-cell, split or twinned crystal, etc.

ADVANCED – Not too much to do here. You can edit your refinement procedure and save it to your user profile. Recommended only for the experienced user or the site administrator.

4. PREDICT – The most powerful tool in the assign unit cell menu for determining crystal quality and confirming the unit cell. I recommend using this very early on if you have any questions about the crystal's quality.

1. Choose about 20 images to predict on and set the mosaicity to 1 (or so). Run.

2. After the first image is displayed, choose the overlay option on the image toolbar (labeled MAX, to the right of the right arrow).

a. At the bottom of the pop-up menu set the sequence start number to the number of the first image you used in the predict spots menu. Set the number of images to equal the number of images you predicted. Run. A new image will be displayed that has all the images on top of each other.

b. Set your reflection circle size (the button with the bubbles) to a small number so that you can see where the predicted reflection is.

c. Adjust you mosaicity if it looks like you have too many or too few reflections and re-run predict.

d. Look very closely and make sure that the prediction matches the reflections you see. If it does not, there is a good chance the unit cell is wrong or there are problems with the crystal, as mentioned above in the REFINE section.

5. INTEGRATE REFLECTIONS

1. Resolution: Set maximum and minimum resolution to 0, the program will automatically set the resolution to include the entire image window during integration.

2. Box: Box sizes should be set to a similar size as was used for FIND SPOTS, if you set it to 0, it will automatically be set to 6X the size of the spots found in the FIND SPOTS process.

3. The rest can be left at the defaults values from installation.

6. .SCALE AND AVERAGE

Main:

1. Reflection list: Select dtintegrate.ref.

2. Exclude Sigma: The default value of 3 will exclude reflections which have about a 99% chance of being an outlier.

3. Rejection Sigma: The default value of 10 will normally suffice, however it can be raised to any value if you are rejecting a large number of reflections.

4. Algorithms:

a. Batch scaling uses simple batch scaling to model all incident beam absorption, decay, etc.

b. B-factor applies temperature dependent scale factors to the data.

c. Absorption correction: Currently 3 methods exist, Spherical 4,3 tends to apply a better correction to small molecule data the others. If it fails, choose another method and see if it succeeds. If none work, your sample may not have required an absorption correction.

5. Error Model: This is probably the hardest part to get down to a simple explanation. There is no "canned" method for doing this.

a. Weight Multiplier: This multiplies the standard deviations by the value set.

b. Weight Addend: This adds a systematic value to the standard deviations.

The idea here is to adjust these parameters to get a relatively flat χ^2 value between 0.8 and 1.2 over all the resolution regions of data. Experience has shown that the Weight Multiplier is specifically dependent on the instrument. Typically between 2 and 3. The Weight Addend can normally be set to the R-merge of the data.

Advanced:

1. Absorption Correction Outlier Sigma: The default value of 125 tends to suffice. In the event that the absorption correction fails, this number can be raised for very strong absorbers to see if it allows a successful absorption correction.

2. Resolution: These can be left at 0 unless you want to cut off poor data at high angles.
3. Scaling Constraints Only available when absorption is not checked. The default values should suffice.
4. Optional Output: Uncorrected, Unaveraged Reflections with Correction Factors should be selected, with an output file name of f2plus.dat, to be imported into teXsan or CrystalStructure. When an absorption correction is not applied or fails, the Corrected, Unaveraged Reflections should be selected, with an output file name of f2.dat and the Output hkl, I, SigI, No Header box checked, to be imported into teXsan or CrystalStructure.

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1 About this Manual

What You Should Know

This manual is a user guide for *CrystalClear*, the instrument control and processing software that is a companion to the Rigaku R-AXIS and Rigaku Mercury and Jupiter CCD Automated X-ray Imaging Systems.

To effectively use this software, you should be familiar with:

- Your detector equipment and how it operates

- Crystallography techniques and terminology
- Windows NT or Windows 95/98

How This Manual Is Organized

The manual includes the following sections:
About this Manual: This is the section you are reading now. It gives an overview of this manual.
Installation: This section details how to install the *CrystalClear* software.
Introduction to CrystalClear: This section gives an overview of *CrystalClear's* user interface.
Running *CrystalClear* for the First Time : This section discusses how to log in to *CrystalClear* for the
first time, and how to set up your initial project and sample.
Common CrytalClear Tasks: This section gives brief overviews of the common scenarios of collecting
data and processing data.
Data Collection and Processing: This section covers the process of collecting and processing data in
more detail.
Command Reference: This section gives information about peripheral features of *CrystalClear* such as
managing projects and samples, displaying the processing state, etc.
Additional Processing: This section covers how to create macros, new collection schedules, and merge
reflections.
Images: This section gives an overview of the Image window and how to use it.
Appendix: The Appendix includes information about *CrystalClear's* directory structure, administrative
functions, and log file information. It also includes a troubleshooting section that lists common problems you may encounter in *CrystalClear*, and how to correct them.

Notation Conventions

Throughout this manual, we will use consistent notation conventions:
- Product and program names are set in *Initial Cap Italic* type.
- Directory names and filenames are set in `monospace` type.

- Code listings are set in `monospace` type.
- Menu options, dialog options and field names are set in **bold**.
- Instructions for choosing menu items will include a > between items.

For example: Choose **File > New**.
- Keystrokes are displayed in parentheses. For example: Press (Enter).
- A plus sign between keys indicates that the keys should be pressed at the same time.

For example: Press (Ctrl+C) to copy the selected text.
- Instructions for using the mouse to select dialog buttons or toolbar buttons, or to select items in a graphical display will read:

Click the **Start** button.
or
Click and drag the mouse pointer to select the desired spot.

Reflection Lists

CrystalClear reflections lists are saved as ASCII files. The first line consists of 3 fields telling the number
of integer, float and string values for each reflection. The next lines are the field labels as character strings for each integer, float or string value: the first three fields are H, K, and L (integers); the next two
are intensity and sigma (floats); the rest are optional. Field labels cannot contain white spaces (spaces,
tabs, etc.) and should begin with n (for integer), f (for float), or s (for string). After the field labels are listed the reflections, one per line in free format.
For example, the first lines of a reflection file follows:
4 7 1
nH
nK
nL
fIntensity
fSigmaI
fObs_rot_mid
fObs_rot_width
fResolution
fLPfactor
fCorrelation
sBatch
22 -1 16 3566.77 121.549 … 1001
4 integers, 7 floats, 1 string
3 integer field labels
7 float field labels
1 string label
actual reflection file with 3 integers, 7
floats (2 shown), and one string

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CrystalClear/d*TREK Coordinate System

The d*TREK default laboratory coordinate system shown in the next figure is defined as follows:
1. The origin of the laboratory is at the crystal.
2. The **X** axis goes from the crystal toward the goniometer baseplate. ***This may be horizontal, vertical or neither.***
3. The **Z** axis goes from the crystal toward the source.
4. The **Y** axis make a right-handed system after **X** and **Z** are chosen.
5. All positive hardware rotations are right-handed.
6. The crystal to detector distance is positive even though it is usually at a negative Z value.
7. The direct beam position on the detector in pixels is specified when the detector is perpendicular to the source (rotations are at zero) AND the detector translations in X and Y are zero. In the actual experiment, the detector may be rotated or translated away from this position.
The following text lists the 19 different properties that can be refined or fixed.

Crystal

All crystal Crystal cell (lengths and angles), orientation and mosaicity
All cell Cell lengths and angles
All lengths Cell lengths a*, b*, c*

a* Cell length a*
b* Cell length b*
c* Cell length c*
All angles Cell angles α*, β*, γ*
alpha* Cell angle α*
beta* Cell angle β*
gamma* Cell angle γ*
All rots Crystal orientation angles
Rot1 Crystal orientation angle around X
Rot2 Crystal orientation angle around Y
Rot3 Crystal orientation angle around Z
Mosaicity Crystal mosaicity
Detector
X
Detector
Z
Y
Source
Goniometer baseplate

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All detector All detector translations and rotations
All trans Detector translations along X, Y, Z
X/Trans1 Detector translation along X
Y /Trans2 Detector translation along Y
Dist/Trans3 Detector translation along Z
All rots Detector rotation around Z, X, Y
Rot1 Detector rotation around Z
Swing/Rot2 Detector rotation around X
Rot3 Detector rotation around Y
Source
Wavelength Source wavelength
All rots Source vector rotations around X & Y
Rot1 Source vector rotations around X
Rot2 Source vector rotations around Y

Related Documentation

For more information on the image collection device that you will be using with *CrystalClear*, see the
user guide that came with the device. Currently, *CrystalClear* collection tasks support the Rigaku RAxis,
and Rigaku Mercury and Jupiter CCD Automated X-ray Imaging Systems. *CrystalClear*
processing supports the Rigaku R-Axis, and Rigaku Mercury and Jupiter CCD Automated X-ray Imaging
Systems. In addition, *CrystalClear* processing supports Bruker, MAR CCD, MAR IP, ADSC CCD, MacScience, Brandeis CCD, and MedOptics images.
You can also check the Molecular Structure Corporation web site for product information, application
notes, service bulletins, and on-line documentation. Set your browser to http://www.msc.com.

2 Installation

System requirements

To run *CrystalClear* you will need the following:
Imaging System Rigaku R-AXIS IV or Rigaku Mercury or Jupiter CCD Automated X-ray Imaging Systems
Computer System Pentium 450 MHz or better (500 MHz recommended)
Memory Minimum 384 Mb RAM (512 Mb recommended) for R-AXIS
Minimum 256 Mb RAM (512 Mb recommended) for CCD
Available hard drive space Minimum 50 meg hard drive space for the *CrystalClear* program, plus additional space as needed for your data storage
Pointing Device Mouse
Video System 1280 by 1024, 256 color capability or better
19 inch monitor (21 inch recommended)
Operating System Windows NT 4.0 with Service Pack 3 (recommended), or Windows 95/98
Drive CDROM Drive
Parallel (LPT) port A parallel (DB25) port to accommodate the Crypto-Box dongle

Installing the Crypto-Box Dongle

CrystalClear comes with a Crypto-Box dongle. This Crypto-Box must be installed on the same computer
where *CrystalClear* is installed. The Crypto-Box works transparently with *CrystalClear* to prevent unauthorized use and distribution of *CrystalClear*.
To install the dongle,
1. Detach printer (if any) from the parallel port.
The parallel port is a DB 25 port that is normally located on the back of the computer. It is a female connector with 25 holes that match up with pins in the male end of the dongle.
2. Plug the male end of the dongle into the parallel port and tighten the screws.
If the computer has more than one working parallel port, you may attach the dongle to either one.
3. If needed, reattach the printer to the female end of the dongle.

Installing CrystalClear

To install *CrystalClear*,

1. Place the *CrystalClear* CD in your CDROM drive.
2. Click the **Start** button, then click **Run**.
3. Enter *d:\setup*, where *d* is the drive letter of your CDROM drive, then press (Enter).
The **Welcome** dialog will appear.
4. Click **Next** to continue.
5. The license agreement will be displayed. Read the license agreement and click **Yes** to continue with
the installation.
6. The INFOLIST.TXT file will be displayed. This document includes important information about *CrystalClear*, including release notes for the current version, and other information that may not be included in the user manual. Click **Next** after reading the material.

7. In the **Select Destination Location** dialog, select the location where you want the *CrystalClear* files
installed. The default location is *C:\PROGRAM FILES\RIGAKU MSC\CRYSTALCLEAR*. We suggest using the default location, but if you prefer to install *CrystalClear* in a different location, modify the path and click **Next**.
Follow the remaining prompts until the *CrystalClear* installation program is completed. See *Appendix A: Files and Directory Structure* on page135 for information on the files that are installed, and the directory structure that is created during the installation.

After installation

Installation

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After you have installed *CrystalClear*, log on as "administrator" and set up the users and system configuration. See *Appendix B: Administration* on page 141 for detailed information on administrative
functions. You should also make sure that the Rigaku R-AXIS or Rigaku Mercury or Jupiter CCD Automated X-ray Imaging System that *CrystalClear* will be working with is set up correctly.

Uninstalling CrystalClear

To uninstall *CrystalClear*,
1. Click the **Start** button on the Windows Task Bar.
2. Select **Settings > Control Panel**.
3. In the Control Panel, click **Add/Remove Programs** .
The **Add/Remove Programs Properties** dialog will appear.
4. Locate **Rigaku/MSC CrystalClear** in the list and double-click.
CrystalClear and all its components will be removed. Any image files you may have, and data files that were created or processed by *CrystalClear* will not be removed from your system.

Introduction to CrystalClear

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3 Introduction to CrystalClear

What is CrystalClear?

CrystalClear is a software program designed to work with the Rigaku R-AXIS or Rigaku Mercury or Jupiter CCD Automated X-ray Imaging Systems for the collection and processing of crystal data. *CrystalClear* interfaces with the X-ray imaging system to collect data, then will process that data. *CrystalClear* can be used to process data that may have been collected previously. It can support .IMG
(CCD), .OSC (RAXIS), and .STL (RAXIS) image files. *CrystalClear* can also support Bruker, MAR CCD, MAR IP, ADSC CCD, MacScience, Brandeis CCD, and MedOptics images.

Overview of the CrystalClear Interface

The *CrystalClear* interface, pictured above, contains several elements that let you control collection and
processing. The items below refer to the numbers in the display above.
1 Task drop down list
2 Current sample
3 Run mode
4 Flow bar

5 Step within the selected task
6 Substeps of a step
7 Toolbar
8 Image window
9 Command Bar
10 Message Window
11 Status Bar

Task Drop-down List

The Task drop-down List displays the currently selected task. Display the list by clicking the drop-down
button. Specific tasks will be discussed in later sections of this manual. Tasks include**: Screen Collect**
and Process, Collect and Process, Collect, Process, Combine Reflections

Current Sample

CrystalClear allows one open or current sample at a time. After **Login**, the sample most recently opened
is automatically displayed in an Open Sample dialog. The user may wish to open this sample or create a
New Project or **New Sample**. Alternately, to open a current sample, click **File > Open Sample** . To start a new sample, click **File > New Sample** . If a new sample is created when sample is current, *CrystalClear* automatically saves and closes the existing. Upon exiting *CrystalClear*, the current sample
is automatically saved and closed

Run Mode

The **Run Mode** buttons allow you to choose whether you want to process your data in automatic mode
or manual mode. The **Auto** will allow *CrystalClear* to process the data with current settings, without user intervention. Click **Abort** to stop the **Auto** feature if you wish to manually process your data step by
step.

Flow Bar

The *CrystalClear* interface is designed to help the user complete the tasks of collecting and processing
crystal data by following the steps displayed on the Flow Bar. The Flow Bar displays the current task,
and all the steps required to complete that task. As you move through the steps in the task, the current step button will change to yellow. Note that the steps in the Flow Bar change depending on the **Task** selected from the drop-down List.

Step Button

A button represents each step in the task. When you click the button, a dialog will be displayed with information pertinent to that step. You can make adjustments to the settings, then click the **Run** button
on the dialog to continue.
When a step is running, the button will be yellow.

Steps with Substeps

Step buttons that have a small arrow to the left of the button label include substeps. Click the button to
display the substeps. Clicking the step button again will collapse the list, so the substeps are no longer
displayed.

Toolbar

The Toolbar includes buttons needed to complete common activities. Some of these include: selecting a
processing algorithm, toggling display items, moving through images, etc.
As you move your mouse cursor over each button, a Tool Tip will appear that describes the button's function. Note that these functions are also available on the menu.

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New Sample
Open a Sample
Save Sample
Use d*TREK as the processing module
Use TwinSolve as the processing module. When you choose this option, CrystalClear automatically uses a mix of processing modules. TwinSolve is selected for the Index algorithm, while d*TREK is selected as the Integrate and Scale algorithms. (available only with CCD)
View Image Collection updates. When toggled on, image updates will be displayed during collection.
View Image Processing Updates. When toggled on, processing results will be displayed during processing.
View Image
Show Processing State Display. A dialog displaying the processing state will be displayed.
Show Scan State Display. A dialog displaying the scan state will be displayed.
Show Instrument State Display. A dialog displaying the instrument state will be displayed.
Show Manual Instrument Control
View Log File. The Open dialog appears, allowing you to select the .LOG file to view. That file is then opened in the Log File Editor
Set Resolution
The RAX Shape crystal viewer will be displayed. This is available for CCD instruments only.
Previous Window. The previous window will be displayed.
Next Window. The next window will be displayed.
About. The About dialog will be displayed.
Toggle Task List. The task List on the toolbar will be toggled on and off as you click this button.

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Toggle Standard Tools. The standard tools on the toolbar will be toggled on and off as you click this button.
Toggle Flow Bar. The Flow Bar display will be toggled on and off as you click this button.
Toggle Command Bar. The Command Line display will be toggle d on and off as you click this button.

Toggle Message Bar. The Message Bar display will be toggled on and off as you click this button.
Toggle Status Bar. The Status Bar display will be toggled on and off as you click this button.
Toggle Script Tools. The Script Tool button display will be toggled on and off as you click this button. The Script tool buttons are:
Play
Record
Pause
Stop
Scripting is not fully implemented in CrystalClear.
Shutter Status (open or closed)
Close the shutter and shut down the device driver or processing server immediately.
Processing and Collection Status. The cube rotates when data is being collected or processed.

Execute Step Button

You can immediately execute a particular step by clicking its **Execute Step** button. This is the small button on the right of the large button with the Lightening icon.
Normally, when you click a step button, a dialog is displayed, allowing you to change parameters, then
you click the **Run** button to start the process. Clicking the **Execute Step** button starts the process without displaying the associated dialog. The current values are used for the processing.
When the process for a particular step is running, the **Execute Step** button is displayed with a red X. You can click this button to stop the process.

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Next Step arrows

The **Next Step** arrows indicate the next step in the task. This arrow will change to a Decision Point or
Stop Sign when further action is required. You can also click the **Next Step** arrow to change it to a Decision Point or Stop Sign. You can pause the current processing by changing the Next Step arrow to a
stop sign.

Decision Points

Whenever you must make a decision on what direction to go next, a decision point icon will appear below the current step. Arrows leading from the decision point icon will point to the next step for each
possible choice. Click the decision point icon to open the decision dialog, then select the next step. Alternatively, you can click one of the buttons to which the Decision arrows points.

Stop Signs

You can click the Next Step arrow until it becomes a Stop Sign. When a Stop Sign icon appears below a
step button, *CrystalClear* is paused at that step and is awaiting the user to click again to resume processing.
You may want to set a stop sign after a specific sub-step in the Flow Bar, so that processing pauses after
that step.

Image window

In the Image window, the data images will appear as they are processed. See *Section 9 Images* on page
131 for more information about this window.

Command Bar

The **Command Bar** displays the commands sent to the compute server (d*TREK). In a future release
you will be able to enter commands on the **Command Bar** directly, allowing you to bypass the graphical
user interface if you desire.

Message Window

In the **Message Window**, *CrystalClear* will display various messages informing you of the progress of
the current process.

Status Bar

As you scroll through menu items, a brief description of the selected menu item is displayed on the status
bar.

Log File window

The log file window (not pictured above) displays the contents of a log file. Log files are created with each process in *CrystalClear*. You can display the log file by clicking the View Log File button on the
tool bar, or by selecting View > Log File from the menu. See *Appendix C: Sample Log Files* on page 161 for more information on log files.

4 Running CrystalClear for the First Time

Starting CrystalClear and Logging in

Once *CrystalClear* is installed and your administrator has created a user account, you can start *CrystalClear* and Log in to begin working on your crystal samples.

Before you are able to log in to CrystalClear*, your administrator must create a user account for you. You will receive a* **Login Name** *and a* **Password**. *For convenience, your* **Login Name** *could be the same name used for your system login. If you do not know your user name and password, see your* CrystalClear *administrator.*

Important*: CrystalClear will not run without the Crypto-Box (dongle) installed on the parallel port of the computer. Before starting* CrystalClear*, make sure the dongle (Crypto-Box) is installed.*

To start *CrystalClear*,

1. Click **Start** on the Windows task bar, then select **Programs > Rigaku MSC > CrystalClear**.
The *CrystalClear* program will start, and the Login dialog will be displayed. The current system login user name will automatically be displayed in the **Login Name** edit field.

If CrystalClear *is not on your Start menu, see your* CrystalClear *administrator.*

2. Enter **Login Name**, then press (Tab).

User names and passwords are not case-sensitive.

3. Enter the password, then click **OK**.

Creating Your First Project and Sample

When you log into *CrystalClear* for the first time, the Project Wizard will lead you through the creation
of a new project and sample.
A *Project* is a collection of related samples. For example, you may grow ten myoglobin crystals, which
you plan on processing as individual samples. You can create a project called Myoglobin, then create ten
samples in that project, one for each crystal.
A *Sample* is roughly equivalent to the data collected and processed from one individual crystal.
1. In the **Project Name** field, enter a name for your new project, then click **Next**.
2. In the **Sample Name Wizard** dialog, enter a name for your new sample in the **Sample Name** field,
then click **Next**.
3. In the **Task Selection Wizard** dialog, select a task from the **Task** drop down list, then click **Next**.

This chart shows the tasks on the dropdown menu by clicking the **Task** *down arrow*..

Screen Collect and Process
This task allows you to screen crystals by collecting initial images, decide to collect a data set on a crystal, help determine a data collection strategy, collect the data, and process the images. The software is designed to have one data set per "sample."

Collect and Process
This task allows you to go directly to data collection and process the images once they are available.

Collect This task allows you to only collect data. This option is used when the intention is to process the images at a later time.

Process This task allows you to process already-collected images.

Combine Reflections
This task allows you to combine reflection files from different data sets.

Next, the **Image Files** dialog appears. If you are using existing image files to **Process** a sample, you may specify one image file in the **Image File** path. *CrystalClear* will include all image files in the same location for the sample. If you **Collect** images for this sample, specify the path to store images upon collection. Collected images may be stored in a separate location as the Project and Sample data.

Note: Each time a **New Project** or **New Sample** is created, CrystalClear creates new folders on your

system, located in the assigned path. For example, when a **New Project** named Myoglobin and a **New Sample** named Myo1 is created, CrystalClear creates a folder called Myo1 nested within a folder called Myoglobin (project). Each time a **New Sample** (i.e. Myo2, Myo3, Myo4, etc.) is created within the Myoglobin Project, a new folder for each sample is nested within the Myoglobin folder.

Note: *CrystalClear* automatically stores Project and Sample data to the default location C:\Program Files\RigakuMSC\CrystalClear\data\(Login Name). During user set-up, your administrator may assign a unique path for each user to store Project and Sample data. It is not recommended that administrators use this directory for user base directories! Additionally, it is not recommended that the same directory be used by different users.

4. Click **Finish**. The project and sample will be created. Later, you can add more samples to the same project, or you can create additional projects as needed.

Each **Project Name** *is unique for a* **Login Name**. *To access a specific Project, a user must use the same* **Login Name** *as was used when the Project was created.*

5. Now that you have logged in and created your first project and sample, you can begin collecting and/or processing data.

At your next **Login**, the **Open Sample** dialog will display the most current sample. *CrystalClear* allows only one open or current sample at a time in each *CrystalClear* window. The user may wish to open this sample or create a **New Project** or **New Sample**. Alternately, to open a current sample, click **File** > **Open Sample**.

To begin a new sample, click **File > New Sample** . If a new sample is created when sample is current, *CrystalClear* automatically saves and closes the existing current sample.

Upon exiting *CrystalClear*, the current sample is automatically saved and closed. See *Section* 7 Tool Reference on page 93 of this manual for more information on adding new samples.

5 Common CrystalClear Tasks

This section gives a brief overview of several common *CrystalClear* tasks. In later sections, each task is

discussed in more detail with explanations of parameters, preferred procedures, etc.

Collect Images

CrystalClear can be used to collect images of your crystals on the Rigaku R-AXIS IV, or Rigaku Mercury or Jupiter CCD Automated X-ray Imaging Systems.

To collect images,

1. Start *CrystalClear* and enter **Login Name** and **Password**.

When a **Login Name** *is used for the first time,* the **Project Wizard** will lead *the user through the creation of a new project and sample. See* Section 4 Running CrystalClear for the First Time *on page 27, if you need assistance.*

When a **Login Name** *is repeated, the Open Sample dialog allows the user to open an existing Project, or begin a new Project. The last project and sample used (for the Login Name) will be listed as default.*

2. At the **Open Sample** dialog, select the **Project** and **Sample**.

3. Select **Collect and Process** from the **Task** drop down list, then click **OK**.

The **Open Sample** *dialog allows the user to begin a* **New Project** *or a* **New Sample** *by clicking the appropriate buttons.*

The **Setup** dialog will appear.
4. Check the values on each tab of the **Setup** dialog box, adjusting any values as desired, then click **OK**.
5. When prompted to **Initialize** the device, click **OK**.
6. Mount your crystal. At the **Mount Crystal** prompt, click **OK** when ready.
7. If you are using the Mercury CCD, the shape program will open. Draw the faces of the crystal to be
used in the Numerical Absorption Correction.
8. When the **Collect Images** dialog box appears, choose a collection schedule and then click **Run**.
To watch the progress of the collection, click the ***Show Instrument State Display*** *button on the toolbar.*

Process Images

Once images have been collected, you can use *CrystalClear* to process them. If you selected **Screen Collect and Process** or **Collect and Process** as your task, the *CrystalClear* Flow Bar will automatically
begin the **Process** steps when collection is complete. If you have previously collected the images to Process, continue with the following steps.

Setup

The first step in the CrystalClear Flow Bar is **Setup.**
1. Start *CrystalClear*. Enter **Login Name** and **Password**

Common CrystalClear Tasks

When a **Login Name** *is used for the first time,* the **Project Wizard** will lead *the user through the creation of a new project and sample. See* Section 4 Running CrystalClear for the First Time *on page 27, if you need assistance.*
When a **Login Name** *is repeated, the Open Sample dialog allows the user to open an existing Project, or begin a new Project. The last project and sample used (for the Login Name) will be listed as default.*
2. At the **Open Sample** dialog, select the **Project** and **Sample**.
3. Select **Collect and Process** from the **Task** dropdown menu, then click **OK**.
The **Open Sample** *dialog allows the user to begin a New Project or a New Sample by clicking the appropriate buttons.*
The **Setup** dialog will appear.

Common CrystalClear Tasks

4. Check the values on the different tabs of the **Setup** dialog box, change any values that are not correct
and then click **OK**. In particular, pay close attention to the necessary parameters **X and Y Direct Beam positions, Crystal To Detector Distance, Detector 2q, and Source Wavelength**.
The CrystalClear Flow Bar will automatically begin the next step, **Assign Unit Cell**. The **Find Spots** dialog will appear.

Assign Unit Cell

The next step in the Flow Bar is Assign Unit Cell. This step in the Process assists the CrystalClear user
in procedures Find Spots, Index Spots, Refine Cell, and Predict Spots. The purpose of this section is to
determine and confirm the unit cell and mis-setting angles.

Find Spots

1. The **Find Spots** dialog allows the user to select images. Image numbers may be entered manually or
selected from a list.
When entering image numbers manually, be sure to use a dash (-) to separate consecutive image entries or use a comma (,) to separate non-consecutive images entries. Before clicking the **Run** button to **Find Spots**, de-select (un-highlight) the **To Use** entry field to verify the selected image entries.

Common CrystalClear Tasks

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Right-click an entry field for further menu options as follows:
View Images List Displays a list of image files
Select Scan Allows user to select images of a scan
Clear Scan Clears selected images of a scan

Common CrystalClear Tasks

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In the **View Images List**, all images available are listed with a sele ction box in front of the image name
and the type of rotation/oscillation with its beginning and end angles following. Click on the box to select/deselect the image. The sequence field dynamically changes with the selections.
View Images List *menu option (right click on entry field)* allows the user to select image files. Before clicking the **Run** button to **Find Spots**, de-select (un-highlight) the **To Use** entry field to verify the selected image entries.

Common CrystalClear Tasks

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2. If desired, change other parameters in the **Find Spots** dialog box.
3. When satisfied with the settings, click **Run**.
CrystalClear *finds the spots in each image file selected, creating a reflection and log file called dtfind.ref and dtfind.log, respectively. Each image appears in the image window as it is processed.*

Index Spots

The CrystalClear Flow Bar will show the next step of **Assign Unit Cell**. Click **Index Spots** on the Flow
Bar. The **Index Spots** dialog will appear.
The **Index Spots** dialog allows the user to index the spots from a reflection file, and thus assign the unit cell. This can be done either automatically with judicious setting of the parameters or interactively with the "**User Chooses Solution**" option.
1. The **Index Spots** dialog allows the user to index the spots from a reflection file, and thus assign the
unit cell. This can be done either automatically with judicious setting of the parameters or interactively with the "**User Chooses Solution**" option.
2. If desired, change parameters in the **Index Spots** dialog box.
3. When satisfied with the settings, click **Run**.
CrystalClear *indexes the spots from the reflection file selected, updates the database for this sample, and generates a log file called dtindex.log. If "User Chooses Solution" is checked, the user must choose one of the crystal lattice solutions displayed by double clicking on the row in an* **Index Results Window**.

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4. Look over the **Index Results** to identify the cell in question. Least Squares Residuals (LSR) represent the residual between the current cell and the triclinic cell (lower is better). Depending upon the degree of accuracy of your detector geometric parameters, the LSR will vary (very small is well known.)
Select a solution, if it is not already selected.
5. Click **OK**
The **Processing State Display** *may appear. It shows the current parameters for the sample. For more information on the* Processing State *see page 98 of* Section 7 Tool Reference.
For more information, see Index Spots *on page 63 of Section* 6 Data Collection and Processing.

Refine Cell

The CrystalClear *Flow Bar will automatically begin the next step* within **Assign Unit Cell**. *The* **Refine**
Cell *dialog will appear.*
1. The **Refine Cell** dialog allows the user to refine the crystal, detector, and source parameters.

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2. Select the desired **Macro** to use for refinement.
***Macro** is initially set to **Single Step Refine.** The user may use an alternate Macro, however, this setting returns to the default, **Single Step Refin**e following each **Run**.* To create custom macros, click **Advanced** button.. *See Section 8 Additional Processing* on page 119 for information on creating your own macros.
3. Consider adjusting the resolution in the **Resolution Min** and **Max** fields. Adjusting the value in the
peak intensity inclusion criterion in the **I/s (I)** field will allow more reflections in the refinement; or consider adjusting the rejection tolerances in the **X, Y and Rot** fields.
4. Click **Run** to refine with current settings.
When the refinement is finished, the fields in the dialog will be populated with values.
5. Make any desired changes in the **Refine** dialog. Selecting boxes will include a parameter in a refinement. Deselecting boxes will withdraw a parameter from the refinement.
Click **Run** to repeat the refinement, if desired.
Remember, **Macro** *resets to the default,* **Single Step Refine** , *following each* **Run**.
6. If **View Image Processing Updates** icon is toggled on, the reflection in the reflection file will be represented on each image using one of the following colors: included blue circles, excluded green circles, and rejected red circles. Adjusting **Resolution Range** fields, and **I/s** will include/exclude reflections. Adjusting the rejection limit, (X and Y in mm, Rot in Degrees) will include/reject peaks). Also displayed on each peak is a vector representing the difference between the peak top on the image and the center of the predicted reflection related to the current values of the orientation matrix.

Common CrystalClear Tasks

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7. Click **Close** when you are satisfied with the Refine results.

Predict Spots

The CrystalClear *Flow Bar will show the next step within* **Assign Unit Cell**. Click **Predict Spots** on the
Flow Bar and the **Predict Spots** dialog will appear.
1. The **Predict Spots** dialog allows the user to select images to predict reflections. Image numbers may
be entered manually or selected from a list.

*When entering image numbers manually, be sure to use a dash (-) to separate consecutive image entries or use a comma (,) to separate non-consecutive images entries. For example, you can enter images such as 2-5, 7, 9-12. Before clicking the **Run** button to **Predict Spots**, de-select (unhighlight) the **To Use** entry field to verify the selected image entries.*
Right-click the "To Use" field for further menu options as follows:
View Images List Displays a list of image files
Select Scan Allows user to select images of a scan
Clear Scan Clears selected images of a scan
In the **View Images List**, all images available are listed with a selection box in front of the image name and the type of rotation/oscillation with its beginning and end angles following. Click on the box to select/deselect the image. The sequence field dynamically changes with the selections.

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2. Make other adjustments to desired settings.
3. Click **Run** to predict spots.
CrystalClear *predicts the spots in each image file selected, creating a log file called dtpredict.log. If the view Image Processing Updates icon is toggled on, predicted spots are represented by colored circles on the image(s). The predicted pattern should closely match the observed pattern.*
For more information, see Index Spots on page 63 of Section 6 Data Collection and Processing.

Strategy

For detailed help, see Strategy *on page 80 of* Section 6 Data Collection and Processing.
Strategy can be used to automatically generate a collection schedule so you don't have to.
1. Click **Strategy** on the flow bar.
The **Strategy** dialog will appear.
2. Make changes in setting, if desired.
3. Click **Run**.

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Integrate Reflections

For detailed help, see Integration *on page 83 of* Section 6 Data Collection and Processing.
Once the reflections can be accurately predicted, they can be integrated.
1. Click **Integrate Reflections** on the flow bar.
The **Integrate Reflections** dialog will appear.
2. The **Integrate Reflections** dialog allows the user to select images. Image numbers may be entered manually or selected from a list.
*When entering image numbers manually, be sure to use a dash (-) to separate consecutive image entries or use a comma (,) to separate non-consecutive images entries. For example, you can enter images such as 2-5, 7, 9-12. Before clicking the **Run** button to **Integrate Reflections**, de-select (unhighlight)*
*the **To Use** entry field to verify the selected image entries.*
Right-click the "To Use" field for further menu options as follows:
View Images List Displays a list of image files
Select Scan Allows user to select images of a scan
Clear Scan Clears selected images of a scan
In the **View Images List**, all images available are listed with a selection box in front of the image name and the type of rotation/oscillation with its beginning and end angles following. Click on the box to select/deselect the image. The sequence field dynamically changes with the selections.

Common CrystalClear Tasks

3. Make other adjustments to desired settings such as Box Width and Height (6 to 10 times the spots size without overlapping onto adjacent spots more than half way), Images Per Batch (2 to 4 times the mosaicity for macromolecules and 10 to 30 times for small molecules).
5. Click **Run**.
A CrystalClear message may appear. This reminds the user to create a mask file to exclude areas of the detector from consideration in integration due to uncertain intensities resulting from shadows, bad pixels, or detector flaws. Although it is not necessary to use a mask, it is advisable. See **Nonuniformity**
Type *on page 54, a sub-section of* Setup *in* Section 6 Data Collection and Processing
CrystalClear *integrates the reflections for each image file selected, creating a log file called dtintegrate.log. The* ***Integrate Reflections*** *step can take considerable time depending upon: 1) the number of images to be integrated,2) the number of reflections per image, 3) the computer's available memory, and 4) the computer's processing speed*

Analyzing the Data

Once integration is comple ted, data may be analyzed to determine Laue symmetry, centricity, and spacegroup. See *Section 6 Data Collection and Processing* on page 49for detailed help.

Laue Symmetry

1. Click **Laue** on the flow bar.
The **Laue** dialog will appear.
2. Select the **Reflection List** file to use (generally dtprofit.ref).
3. Make other adjustments to settings as follows:

Common CrystalClear Tasks

Max R-merge Tolerance for considering a Laue class present
Highest Laue Symmetry Limits the highest Laue class to be checked.
Only check Laue groups compatible with
current cell
Unchecked, examines all Laue classes
compatible with current cell
Average Bijvoets (Assume 1+ = 1-) Unchecked examines Laue classes desired
4. Click **Run**.
5. Look over the Laue groups and R-merges for the Laue equivalent reflections.
Select the Laue class, if it is not already selected.
6. Click **OK**

Centricity

1. Click **Centricity** on the Flow Bar.
The **Centricity** dialog will appear.

Common CrystalClear Tasks

2. Select the **Reflection List** file to use (generally dtprofit.ref).
3. Click **Run**.
4. Check the evaluation of centricity
Select the correct centricity if it is not already selected
5. Click **OK**

Spacegroup

1. Click **Spacegroup** on the Flow Bar.
The **Spacegroup** dialog will appear.

2. Select the **Reflection List** file to use (generally dtprofit.ref).
3. Make other adjustments to settings including the average intensity **<I/Sig> Tolerance** for the parity
groups.
4. Click **Run**.
5. Evaluate the suggested space group(s).
Crystal 2 tab of the **Set Up** dialog to enter the space group.

Scale and Average

Once integration is completed, you should scale the reflections.
1. Click **Scale and Average** on the flow bar.
The **Scale and Average** dialog will appear.
2. Select the **Reflection List** file to use (generally dtprofit.ref).
2. Make any other adjustments to the settings that you desire. Some items to consider are the level at which you exclude reflections from the refinement (Exclude Sigma) but include in R-merge, the level of which to reject outliers either by the standard deviation (Rejection sigma) or by the Chi Square deviation (based on Maximum or on percentage rejected), the way in which to determine the error model, batch scaling, absorption algorithm (and hence the method of correction), and output of the reflection file.
3. Click **Run**.

A CrystalClear message appears.
*The **Scale and Average Results** window will appear with the results of the scaling displayed as graphs, generating a log file, and writing the reflection file to the sample directory.*
.

6 Data Collection and Processing

There are five basic steps to collecting and processing data with *CrystalClear*. The Flow Bar leads you
through each of these basic steps, with some variations based on the processing algorithm that is selected.
Setup This step allows you to set default parameters for the data collection and processing. The *CrystalClear* administrator can specify many setup values as default values for your entire site. See *Appendix B: Administration* on page 141 for information on setting site default values. Users can also override site defaults for a specific project. This step is not dependent on the selected processing algorithm.
Collect Images In this step, the data is colle cted using *CrystalClear* on your R-AXIS or CCD X-ray detector. This step is not dependent on the selected processing algorithm.
Index Indexing determines the unit cell parameters and orientation of the crystal.
Integrate This step integrates the reflections on the collected images. In this step, the operation required, and the results are dependent on the selected processing algorithm.
Analysis This step helps to determine the Laue class, centricity and space group.
Scale This step performs post-processing analysis and normalization of the collected data. In this step, the processes required, and the results are dependent on the selected processing

algorithm.

Select a processing algorithm

CrystalClear is designed with two processing modules, allowing you to choose the way your data is processed.

The processing modules supported by *CrystalClear* are:

d*TREK

TwinSolve

To select a processing module,

1. Click the toolbar button representing the processing modules you wish to use:

Use d*TREK

Use TwinSolve (available only when processing CCD images)

- *Alternatively, the processing module options are available on the* CrystalClear *menu.*

Click **Sample**>*, then select the processing module you wish to use.*

TwinSolve includes only an indexing algorithm. You should use the solution found in TwinSolve to index a known cell in indexing. If you select TwinSolve, d*TREK will automatically be selected as the algorithm for **Integrate and Scale** .

Setup

The first step in collecting or processing data is to set the parameters to be used in the **Setup** dialog. Once you have selected the sample, the **Setup** dialog will appear. . For processing, it is necessary only to

have the following five fields correct: **X and Y Direct Beam positions, Crystal To Detector Distance,**

Detector 2q, and Source Wavelength. All other parameters are kept inside *CrystalClear* for your use.

Many of the values on the Setup tabs are set as site defaults assigned by your CrystalClear administrator,

or by the user as Project defaults.

- *Alternatively, Setup dialog can be accessed by clicking the* **Setup** *button on the Flow Bar.*
- *The Setup dialog can also be accessed on the CrystalClear menu. Click* **Sample > Setup**.

The Main Tab

The Main tab in the **Setup** dialog includes the basic settings that are most often adjusted during collection and processing of data. A few of the items found on the **Main** tab are also found on the other

Setup tabs, along with additional settings that normally do not change.

Project and Sample: The names of the current project and sample are listed for your reference.

Crystal ID: The Crystal ID is a name or number you can give to your crystal for your personal reference.

This value is not used in collection or processing.

Temperature (º C): The temperature of the crystal sample at the time of collection, in Celsius.

Crystal to Detector Distance (mm): The distance from the crystal to the detector when collecting images.

If you are processing existing images, the value specified when the images were collected will be displayed.

Detector 2q (º): Swing angle of the goniometer. If you are processing existing images, the value specified when the images were collected will be displayed.

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Note: **Crystal To Detector Distance (mm)** *and* **Detector 2q (°)** *fields show the hardware or unrefined*
values. If "per scan" *is displayed in the* **Crystal To Detector Distance (mm)** *field, different scans will have different values. In this case, refer to the* **Scan State Display** *window to see the values for each scanned image.*

The Crystal1 Tab

The **Crystal1** and **Crystal2** tabs include information about the crystal.

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Unit Cell Parameters: The unit cell parameters for the cell.
a (D) default = 50.000000
b (D) default = 100.000000
c (D) default = 150.000000
α (°) default = 90.000000
β (°) default = 90.000000
γ (°) default = 90.000000
Size: The size of the crystal in millimeters.
X (mm) default = 0.2
Y (mm) default = 0.2
Z (mm) default = 0.2
Mosaicity: Specify the starting value to use for crystal mosiacity. The default starting value is 0.6.
Color: Specify the color of the crystal. You can choose from a drop down list of predefined colors, or enter a different color name in this field. The predefined choices are: blue, colorless, gray, green, orange, red, white, and yellow.
Mount: Specify the mounting type used for the crystal. You can choose from a drop down list of predefined mount types, or enter a different mounting type name in this field. The predefined choices are Loop, Capillary, and Fiber.
Morphology: Specify the morphology of the crystal. You can choose from a drop down list of predefined morphologies, or enter another name in this field. The predefined morphology types are: Block, Chip, Chunk, Platelet, and Prism.

The Crystal2 Tab

The **Crystal2** tab contains additional information about the crystal as a continuation of the **Crystal1** tab.

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Spacegroup*:* Specify the spacegroup of the crystal, if known.
Unknown vs. Known Spacegroup: If you know the spacegroup, select **Known Spacegroup**. If you do not know the spacegroup, select **Unknown Spacegroup**.
Specifying a known spacegroup may save time later on as the crystal is processed.
Crystal System: If you selected **Known Spacegroup**, this option will become enabled. You can select from the drop down list of predefined **Crystal Systems** and then scroll through the available spacegroups from the list under **Number** and **Name**, or alternately, type either the number or name in the appropriate **Number** or **Name** field.
Number and Name: To enter a known spacegroup, type either the number or the name in the appropriate field. Alternately, if you know the **Crystal System** and need to be reminded of the possible Space Groups, select the **Crystal System**, then scroll and choose the Space Group from the list under **Number** and **Name**.

Orientation Angles: These values will be calculated later on by *CrystalClear*. Leave them as 0.000000 when starting a new sample.
Molecular formula: Specify the molecular formula for the crystal. You may enter the formula as it appears in your compound. *CrystalClear* will determine the empirical formula for you.

The Detector Tab

The **Direct Beam** settings on the **Detector** tab are based on the type of X-ray detector. Normally, the values are set as site defaults by your CrystalClear administrator. The **Crystal to Detector Distance** may be changed on the **Main** tab of the **Setup** dialog, as well as on the **Detector** tab. The **Rot2/ 2q (°)**
can also be set on the M**ain** tab. The other **Direct Beam** settings on this tab are generally not changed.
The **Non-uniformity Type** group box offers the user several options. The user may choose to create a
mask file to exclude areas of the detector from consideration in integration. Mask are used due to uncertain intensities resulting from shadows, bad pixels, or detector flaws. Although it is not necessary
to use a mask during processing, it is advisable.

- None
- Simple Mask

Simple Scale

- Dark and Mask

Dark, DC, and Mask
Select the desired radio button; then specify the mask filename and/or dark filename. Usually, the software will set these as the occasion permits, such as the creation of a simple mask for integration.

The X-Ray Source Tab

The **X-Ray Source** tab allows you to specify the X-ray source that your system uses. Normally this information is set as site defaults by your *CrystalClear* administrator.
kV: Specify the kV of your X-ray source.
mA: Specify the mA of your X-ray source.
Element: Select the element type of your X-ray source from the predefined drop down list. The possible predefined choices are Chromium, Copper, Gold, Iron, Molybdenum, Silver, and Tungsten.
Wavelength: Specify the wavelength of your X-ray source. The wavelength is based on the Element type. When you select an Element, a valid wavelength will automatically be selected for you.
Source Type: Select the source type of the X-ray source from the predefined drop down list. The predefined choices are Rotating Anode, Sealed Tube, and Synchrotron.
Optics: In this section of the tab, specify the following attributes of your detector:
Type: Select from list: Mirrors, Confocal, Graphite Monochromator, or Multilayer
Focus: Select from a predefined list: 0.1, 0.15, 0.2, 0.3, or 0.5
Slit Size: Specify the slit size
Collimation Type: Specify the Collimation type
Note: Many of the fields contain pulldown menus. Although there are several common items in each list, the user can enter text strings if an option is not present for their experiment.

The Notes Tab

The **Notes** tab provides a small notepad to record notes about a sample. Notes can be stored as site level
data (if you are a *CrystalClear* administrator), or as Project, User or Sample level data. Notes can be accessed at any time by opening the associated project and sample, open the **Setup** dialog, click the **Notes** tab.

Save the Setup

Settings in the Setup dialog are automatically saved with the current sample. Some values may change
as the data is processed.
Setup data can also be saved to the project level data file, or site level data file (if you are a *CrystalClear*
administrator). To save Setup data to the project or site data files,
1. Click Save.
The **Default Manager** dialog will appear.

- *For assistance using the* **Default Manager**, *see page 209 in* Appendix F: Defaults in CrystalClear.

2. Check the desired level to save.
3. Click **OK**.
Note: Site-level defaults are saved to CrystalClearSiteDefaults.ho in the \DATA directory.
User-level defaults are saved to CrystalClearUserDefaults.ho in the *user* directory.
Project-level defaults are saved to CrystalClearProjectDefaults.ho in the *user**project* directory.
A Sample-level default is saved to *samplename*.ho in the *user**project**sample* directory.
Site *level rights are enabled by the* CrystalClear *administrator only.*

Collect Images with an Imaging Plate System (R-Axis IV)

The **Collect Images** dialog prepares a schedule for the collection of data with an Imaging Plate System,
R-Axis IV.
To schedule a collection run:
1. Click the **Collect Images** button on the Flow Bar
The **Collect Images** dialog will appear.

Pixel Size (μ): Select appropriate value.
Readout Area: Select desired entry: Full, Middle, Bottom Half, Custom. Grayed-out options will appear as required: Start Line, Number Lines
Collect Schedules: Assign a schedule in the **Collect Schedules** edit box.
(right click down-arrow) Several common schedules are:
One: 0 (collects one image at $\phi = 0°$**)**
Two: 0,30 (collects one image at ϕ 0°, and one at 30°)
Four: 0,30,60,90 (collects images at $\phi = 0°$, 30°, 60°, and 90°)
Default Screen Schedule
Scan Table: The **Scan Table** contains contains information about scans in columns with headings which can be manipulated. Users are able to **Add**

Scan(s) and **Remove Scan**(s), then make changes to scan settings, as desired.
For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.
Time Estimate: Calculated based on supplied values and number of images.
Required disk space: The amount of disk space required to complete the scheduled collection request.
Total disk space *(drive):* The amount of disk space currently available.
Completeness : Completeness of data in the scan.
Note: If insufficient disk space is available to complete the scheduled image collection request, a CrystalClear warning dialog will appear. The collection request may be cancelled to allow the user to

free more disk space on the system before continuing.
See *Create a Collect Schedule* on page 126 in *Section 8 Additional Processing* for more information about adding your own collection schedule.
2. Use the Scan Table to alter the scans, you may:

- *Use the* **Add Scan** *button to increase the number of scans at a different crystal orientation. Adjust settings as desired.*
- *Use the* **Remove Scan** *button to remove undesired scans.*

For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.
3. Make adjustments to the settings as required.
4. Click **Run** to start the scheduled collection scan.
The **Double-Check Settings** dialog will appear.
5. Review the specified settings on the detector.
6. Click **Start Image Collection**, or **Cancel Image Collection** if an error is found.
In the event CrystalClear detects insufficient disk space available for the entire data collection, a dialog will appear to guide you through selecting a new collection directory. You may need to "cancel" the data collection and free up space on the hard drive. If you wish to delete the images and processing from an old sample (presumably with all necessary file archived), see Delete Projects and Samples *on page 97 of* Section 7 Tool Reference

Collect Images with CCD System (Mercury CCD)

The Collect Images dialog prepares a schedule for the collection of data with a CCD system, the Mercury CCD.
To schedule a collection run:
1. Click the **Collect Images** button on the Flow Bar.
The **Collect Images** dialog will appear.
Dezingered Exposure: Check this option if desired. See the Mercury or Jupiter CCD manual for more information on the Dezinger Exposure feature.
Bin Mode: Select the Bin Mode. See your Mercury or Jupiter CCD manual for more information on the Bin Mode feature.
Collect Schedules (right click down-arrow): Assign a schedule in the **Collect Schedules** edit box.

Scan Table: User may **Add Scan** or **Remove Scan** on the **Scan Table**, then make changes to scan settings, as desired.
For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.
Right-click on any column heading for **All Columns** menu. This allows the user to select (or de-select) individual columns to be displayed (or hidden). Column headings are as follows:
Scan ID: Scan identification number.
Template: Base name of the image.

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*Detector Distance(mm):*Crystal to Detector distance.
2-Theta(deg) 2θ offset of the detector.
Max Resolution: Specify maximum resolution in degrees.
Wavelength:(λ) Specify the wavelength of your X-ray source. The wavelength is based on the Element type. When you selected an Element, a valid wavelength will be selected automatically.
Omega: (ω) The rotation axis on an AFC8 or 9
Phi: (ϕ) Specify the position of the crystal goniometer in degrees, or the rotation axis on the AFC7.
Rotation Axis: Specify Omega (ω), or Phi (ϕ). Omega (ω) used for AFC8 or 9. Omega (ω) and Phi (ϕ), one normally used for the AFC7.)
Start Angle: The angle in degrees of the start position.
End Angle: The angle in degrees of the ending position.
Width: The width of one image, in degrees.
Step: The angular distance between the start angles of two consecutive images in the scan.
Number Images: The number of images to be collected in the scan.
Completeness: The percent completeness of the data in that scan.
Start Number: The start number to assign to the first image of the scan.
Exp Time: Specify exposure time in minutes.
Total Images: Specify total number of images.
Images Collected: Images already collected, if any.
Images Scheduled: Images currently scheduled for collected during next collection run.
Scheduled Start Angle: The angle in degrees of the start position for currently scheduled images.
Scheduled End Angle: The angle in degrees of the ending position for currently scheduled images.
1. Make adjustments to the settings as required.
For example, if you wish to scan 90° of the crystal with a 0.5° image width, and scan every 0.5°, your settings may be:

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Start
Angle
End
Angle Width Step
#
Images

Completeness
Start
#
0.00 90.0 0.50 0.50 180 --- 1
Right-click on column entries to **Propagate** (Down, Up, All). This feature is helpful in setting the same
parameter for several different scans.
Time Estimate: Calculated based on supplied values and number of images.
Required disk space: Amount of disk space required to complete the scheduled collection request.
Total disk space *(drive):* Amount of disk space currently available.
Completeness : Completeness of data in the scan.
Note: If insufficient disk space is available to complete the scheduled image collection request, a CrystalClear warning dialog will appear. The collection request may be cancelled to allow the user to
free more disk space on the system before continuing.
See *Create a Collect Schedule* on page 126 of *Section 8 Additional Processing* for more information about adding your own collection schedule.
3. Click **Run** to start the scheduled collection scan.
The **Double-Check Settings** dialog will appear.
4. Review the specified settings on the detector.
5. Click **Start Image Collection**.
In the event CC detects that the available disk space is insufficient for the entire data collection, a dialog
will appear to guide you through selecting a new collection directory. You may need to "cancel" the data collection and free up space on the hard drive. If you wish to delete the images and processing from an old sample (presumably with all necessary file archived), see Delete Projects and Samples *on*

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page 97 in Section 7 Tool Reference

Index Spots

During the Index phase of processing your crystal data, *CrystalClear* will determine the unit cell parameters. The settings specified in the Setup phase are used as a starting point in indexing the data. Indexing consists of finding spots, auto-indexing and refinement.

Index with d*TREK (RAXIS or CCD)

Find Spots

The **Find Spots** step finds reflection centroids in a single image or a collection of images. The reflection
centroids are written to a file called the dtfind.ref file by default. The found reflection centroids are subsequently used in an autoindexing or refinement step.
In order for autoindexing and refinement to function properly, you should find 50-70 reflection centroids. The exact number needed can vary depending on the centroid accuracy and location in reciprocal space. The prerequisite for finding reflection centroids is knowledge of the properties of the
images from which you are finding reflections.
To find spots,
1. Click the **Find Spots** button in the Flow Bar.
The **Find Spots** dialog will appear.

Select images to be processed. The **Find Spots** dialog allows the user to enter image numbers manually
or select images numbers from a list. Right-click on the To Use entry field to view menu options.

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To enter image numbers manually in the **To Use** entry field, be sure to use a dash (-) to separate consecutive image entries and use a comma (,) to separate non-consecutive images entries. *For example,*
you can enter images such as 2-5, 7, 9-12. Before clicking the **Run** button to **Find Spots**, de-select (unhighlight)
the **To Use** entry field to verify the selected image entries
Right-click an entry field for further menu options as follows:
View Images List Displays a list of image files
Select Scan Allows user to select images of a scan
Clear Scan Clears selected images of a scan
View Images List *menu option (right click on entry field)* allows selection of image files. Before clicking
the **Run** button, de-select (un-highlight) the **To Use** entry field to verify the selected image entries.

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Column 1: Image identification (Check in box denotes image selected)
Column 2: Axis of Rotation - P = phi, C = chi, O = omega
Column 3: Start angle of the image.
Column 4: End angle of the image.
The sequence field changes with the selections.

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2. Specify a **Sigma** level above the average background for a pixel to be considered a peak.
If Sigma is 0, ***Find Spots*** *processes faster because it does not calculate average background and its standard deviation.*
3. Click the **Advanced** tab to set display options.
4. Specify a **Minimum Pixel Value** for a pixel to be considered a peak.
The ***Minimum Pixel Value*** *is compared to non-uniformity corrected pixel values. The actual threshold*
used is the maximum of ***Minimum*** *and* ***Sigma*** *above the average background.*
5. Specify the **Peak filter.**
The Peak size filter is specified as the number of pixels in a 3x3 area that must be above the threshold
*(****Sigma****, **Minimum Pixel Value**) for a peak to be considered a reflection. If spots are large, you might*
want to make this 9. If the spots are small, you might make this 4. ***Peak filter*** *helps distinguish between*
true spots and noise in the images.
6. Select **3D** check box to perform a 3D search to determine peak widths for mosaicity refinement.
By default, a 2D search is automatically performed.
7. Specify the **Padding** to be added.
The padding is the number of images for 3D shoeboxes (in 3D search mode only) at the start and end in

the rotation angle direction. In order to completely contain a 3D peak with a 3D shoebox or volume, pad by 2-4 images and have a ***Box width and height*** *large enough to encompass the reflections. If any*
significant peak intensity is on the edge of a shoebox, CrystalClear *rejects the centroid determined for*

that peak. Thus ***Padding*** *is important to ensure that the peak goes down to background in the rotation*
angle direction.

8. Specify the **Box Width and Height**, in pixels, of the box that appears around each spot in the display.

In either search mode, if these are both set to 0, then CrystalClear will try to determine the box size for
each spot automatically. Of course, this will take extra computational power and time. A good box size
is 6 to 10 times larger than the biggest spot, but without intruding more than half way into neighboring
spots.

9. Specify the **minimum** and **maximum** resolution.

10. When satisfied with your settings, click **Run** to find spots.

The **Find Spots** feature will create the reflection file "`dtfind.ref`," which will be used in the **Index**
Spots step, and the log file `dtfind.log`.

Index Spots

The Index Spots feature indexes reflection centroids in the selected reflection list to elucidate the crystal unit cell dimensions, the crystal orientation, and the Bravais Lattice type.

To index spots,

1. Click the Index Spots button in the Flow Bar.

The Index Spots dialog will appear.

2. If you know the Spacegroup, select the **Known Spacegroup** button, then select the **Crystal System**
from the drop down list.

A ***Spacegroup number*** *of 0 indicates no user preference. In this case, the output header will have the lowest symmetry spacegroup consistent with the selected lattice type.*

3. The **Reflection Lists** box displays the available reflection files. Select the file you wish to use for the
Index Spots procedure.

4. Specify the desired **Resolution** range. If you wish to change the default resolution, click **Set**. See *Set Resolution* on page 119 of *Section 8 Additional Processing* for more information on the **Set Resolution** function.

5. If you wish to select a solution manually, check the **User Chooses Solution** check box. You will be
prompted to select the desired solution from a list of solutions. If not set, the program will automatically select a solution. The number of Bravais Lattices in the list will depend on the value set for **Max Residual** in the **Advanced Tab** (see below).

6. If you wish to set all the values back to the defaults, click the **Defaults** button. You will be prompted to select whether you wish to use **Project** level defaults or **Site** level defaults.
7. Click the **Advanced** tab to set additional values.
8. In the **Max Cell Length** field, specify the maximum cell length in Ångstroms to search.
If this is 0, then CrystalClear *tries to determine a maximum cell length on its own, which is subject to errors.*
9. In the **Max Residual field**, specify the maximum allowed least squares residual for a solution to be

listed.
The program fits the reduced primitive cell to 44 lattice characters. Only those solutions with a residual less than or equal to ***Max Residual*** *are displayed. Typically, residuals greater than 2.5 are not valid solutions. The maximum residual is 100. The default of 2.5 reduces output and helps make it easier to choose the correct solution. If using the Rossman method, a residual of 1 or higher indicates either the wrong solution or misaligned hardware.*
10. In the **Max Vectors** field, specify the maximum number of difference vectors to use in the calculations.
With more difference vectors the calculations take more time and the residuals will be larger. With fewer difference vectors, the calculations take less time and the correct solution may be missed. If 0, CrystalClear *picks a suitable number.*
11. In the **Grid Size** field, specify the grid size in Ångstroms for the direct space Fourier map.
This is not used if ***Use Fourier Method*** *is not selected. If 0, then the program selects an appropriate grid size.*
12. In the I/SigI field, specify the desired value.
13. From the Method drop down box, select a method. The choices are:
1D FFT: The DPS indexing algorithm of Steller, Bolotovsky, & Rossmann[1] is used. About 7300 different directions are examined by an 1D FFT algorithm for whether a principal cell axes is parallel to that vector. Three of the vectors with the most order are selected for cell reduction.
3D Fourier: A 3D cosine Fourier is calculated over a real unit cell volume with grid points x.

$$\cdot = \sum_{p} \cos[2\ (\ *)]$$

where d*(i) is the reciprocal lattice vector for refln_i. Peaks will appear in the Fourier function at the end points of the real cell axes a, b, c and linear combinations of these axes[2].
Reciprocal Space: The reciprocal space method of Sparks is used[3].
Cell reduction used as published by Andrews & Bernstein and Paciorek & Bonin[4].
14. If indexing fails, and you know the correct cell, select the **Use known cell** check box to force the program to look at vectors that match a known unit cell.
Selecting this check box forces the program to look at vectors that match a known unit cell. The unit cell in the header is converted to a reduced primitive cell based on the Spacegroup. The program will search for this reduced primitive cell.
15. Check the **Diffs** check box if desired.

[1] Steller, Bolotovsky, and Rossmann (1997) J. Appl. Cryst. 30, 1036-1040.
[2] Bricogne Proc. EEC Cooperative Workshop on Position-Sensitive Detector Software(1986) 3, 28.
[3] Pflugrath, J. (1997) Method of Enzymology v 276.
[4] Andrews & Bernstein (1988) Acta Cryst. A44, 1009-1018.
Paciorek & Bonin (1992) J. Appl. Cryst. 25, 632-637.

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CrystalClear *can use the vectors calculated from the reflection centroids (e.g. d(i)), or it can use difference vectors calculated from these vectors: d(i)-d(j).*

Difference vectors are useful if the detector position is not well established. Difference vectors can be bad to use if the crystal is twinned or split

16. If **Use Known Cell** is set, select whether to use **Percent Error** or **Absolute Error** within the **Known Cell Parameters/Errors** group box.

*The **Use Known Cell** is set, and the cell errors are specified here. If these are 0, then a 3% error is used.*

17. When satisfied with your settings, click **Run** to index the reflections.

Overcome perceived problems

If there are problems indexing, try the following:

1. Make sure the detector, source and scan properties in the setup dialog are accurate. In particular, make sure the detector translations (i.e. direct beam position on detector, crystal to detector distance) and the scan rotation axis are correct. Make sure the calculated or input **Max cell length** is large enough.

2. Make sure the crystal is not outrageously split, cracked, or twinned. Expose images 90° and 45° away from the original image to double check this.

3. Use a different image or set of images in **Find** to get reflection centroids.

4. Use reflections from more than one image as input to indexing. These images could be 10° or more
separated in rotation angle. Generally, the fewer images used, the better. If the rotation axis is specified incorrectly (i.e. it has a slight tilt not specified in the input header), this could lead to problems. However, small tilts in the rotation axis can be refined in the Refine module.

5. Use 3D reflection centroids from a single wedge (a contiguous set of images) or from more than one
wedge.

6. Use a higher **Sigma** and/or **Minimum** cutoff in **Find**, or select reflections with the Combine Reflections task.

7. Use a different number of **Max diffs** . Both smaller and larger numbers could be tried.

8. Use a different method of autoindexing.

9. Try **Use known cell** if you know the unit cell dimensions.

10. Accept a triclinic cell and refine the detector position, then re-index.

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Refine Cell

The **Refine Cell** feature refines the crystal, crystal goniometer, detector goniometer and source properties in order to reduce the differences between observed and calculated reflection centroids. *CrystalClear* can display the observed and calculated reflection centroids, so the progress and validity of
refinement can be judged.

A header file such as `dtindex.head` or `dtrefine.head` with complete information about the crystal, detector, source, and scan properties is required in order to refine cells (this is created by

CrystalClear). A reflection list with spot centroids such as `dtfind.ref` (from the **Find Spots** procedure) is also required.
A header file called `dtrefine.head` with refined crystal, detector, and source properties is created
by the **Refine Cell** procedure. A scratch reflection list with observed and calculated reflection centroids
that can be plotted by *CrystalClear* will also be created, as well as a script file and an output log file (`dtrefine.log`).
To refine parameters,
1. Click the **Refine Cell** button on the Flow Bar.
The **Refine** dialog will appear.
2. Specify any settings changes, as desired. With the new refinement algorithms, it is recommended that all crystal, detector and source parameters except wavelength be refined initially. It is rare that anything other than this is necessary.

3. If desired, click the **Advanced** button to go to the **Macro Editor** which will allow the user to create
a series of refinement steps varying the parameters refined for each step. This is seldom used and if used
is for extreme cases. We leave it in the software for the exceptional case.
4. Create a new macro by clicking the **New Macro** button.
5. Click **OK** when done.
The **Refine** dialog will return. The **Macro** you created will be in the list of **Macros**.
5. Click **Run** to begin the Refine step.
The refinement process is complete when the number of cycles are completed. If the delta/error, further refinement is needed.

2D *vs.* 3D reflection centroids in refinement

The size and pixel coordinates of reflections will change as they pass through the Ewald sphere due to
crystal mosaicity, source divergence, and source bandwidth ($\Delta\lambda/\lambda$). Thus, the reflection centroids will
be different for 2D data and 3D data. This is illustrated in Figure 1, which shows an 80 by 80 pixel portion of 3 adjacent images of 0.25° rotation width along with an overlay of these images (i.e. 0.75° width). Each image was searched for spots, then ellipses were drawn centered on the observed spot

positions. The overlay shows the shifts in the spot centroids. Thus, the rms errors (lines 80-81 in the output, found in *Appendix C, Refine Spots Log*) from 2D data will be larger than from 3D data. Also, if a
2D reference profile is applied to a partial reflection while integrating with a profile-fitting method, the
reference profile must be oriented properly.

Refinement strategy

The radius of convergence of the refinement algorithm is small so the starting properties should be very
close before trying a refinement. This is usually the case if indexing has given a solution. If the starting

crystal and detector properties are not close to the true values, one might increase the **Rejection Limits**
so more reflections are included in the refinement. However, there is a danger they will be increased too
much and refinement will proceed to a false minimum. It is sometimes better to use only low-resolution
reflections at first because the radius of convergence with them is larger. Then use high-resolution reflections to get the more accurate results. With good reflection centroids, it is best to use all reflections.
The refinement algorithm should be used to refine all parameters from the first. If this is not successful,
it is useful to fix or not refine a property. In the **Refine Window** a checked box means a property is refined, so uncheck the check box to fix the property. Some properties are not refined because of the choice of spacegroup. For example, in orthorhombic cells *a*, *b*, and *g* are not refined. With input reflections found in a single image, the crystal rotation around the source and the detector rotation around the source are correlated, so one of them should be fixed (unchecked). The same is true for the

Overlay of above 3 images.

Figure 1. 2D vs. 3D spot considerations

0.00° - 0.25° 0.25° - 0.50° 0.50° - 0.75°

detector translation along Y and the detector rotation around X (the swing angle). It is a good idea to fix
one of them. With input reflections from widely spaced rotation values, these correlations should not be
a problem. The crystal to detector distance can be refined even with reflections from a single image, especially with a tetragonal or higher spacegroup.
Sometimes refinement works better if you fix most properties and refine only a few at a time. Common
sense should dictate the order of properties that are fixed and refined. For example, if you know the unit
cell parameters from previous work, then *a*, *b*, *c* and *a*, *b*, *g* can be initially fixed. If the detector has just
been moved, refine the detector translations first, then the crystal orientation angles, then the unit cell parameters, then everything. The detector distance should be fixed if there are reflections from a narrow
rotation range and a crystal principal axis is nearly parallel to the source. For any changed settings to take effect, you *must* click **RUN** or **SAVE**.
The refinement scheme used is stored in an output header and is also used during integration. Every few
images (specified by the **Integrate** dialog **Batch** option), the integrated reflection centroids are used to
refine the crystal and detector properties. Thus, the settings of the **Refine** window are important for integration, too.

Predict Spots

The **Predict Spots** feature predicts the reflections that would appear on a range of images. It is typically

used to confirm the results of the refinement step and to better estimate the crystal mosaicity if it was not
refined previously, as would occur if 2D data were used for indexing. Predicted reflections are written to
a file, `dtpredict.ref`.
The **Predict Spots** feature creates a reflection list file with calculated reflection centroids that can be plotted and displayed.
To predict spots,
1. Click the **Predict Spots** button on the Flow Bar.
The **Predict Spots** dialog will appear.

2. Specify the image or images to be processed. To specify a sequence of images, select **Use Sequence**.
Then select the desired images in the **To Use** entry field.
The **Predict Spots** dialog allows the user to enter image numbers manually or select images numbers from a list. Right-click on the **To Use** entry field to view menu options.
To enter image numbers manually in the **To Use** entry field, be sure to use a dash (-) to separate consecutive image entries and use a comma (,) to separate non-consecutive images entries. *For example, you can enter images such as 2-5, 7, 9-12.* Before clicking the **Run** button to **Predict Spots**, de-select (un-highlight) the **To Use** entry field to verify the selected image entries
Right-click an entry field for further menu options as follows:
View Images List Displays a list of image files
Select Scan Allows user to select images of a scan
Clear Scan Clears selected images of a scan
3. Set the **Resolution** range in Ångstroms. If you wish to change the default resolution, click **Set**. See *Set Resolution* on page 119 of *Section 8 Additional Processing* for more information on the **Set Resolution** function. If resolution is set to 0.0 and 0.0, the resolution is set to be the entire resolution possible on the image.
Only reflections that will appear on the detector are predicted, but the resolution range may be restricted further with this option.

4. Specify the desired **Crystal mosaicity**.
If not 0, the specified crystal mosaicity overrides the value found in the input header. In addition, a new header will be written with the updated value for crystal mosaicity.
1. To use a mask, click the **Advanced** tab.
3. Click the **Apply Mask** check box, if desired.
4. Click **Run** to predict spots.
For information on masking, see the erasure tools in Small Image Window Toolbar *on page 134 of* Section 9 Images

Index with TwinSolve (Mercury CCD)

Twinned crystals require special processing to be resolved. *CrystalClear* includes the TwinSolve processing module, which can be use to process twinned crystals.

Find Spots

To find spots,
1. Click **Find Spots** on the Flow Bar.

The **Find Spots** dialog will appear.
2. Select the images to be used to find spots.
You can either select the desired images from the **Image List**, or specify a single range of image sequence numbers in the **Sequence** edit box.
We recommend that you perform a find on all the images from the first scan of data, then repeat the find step using all the images from each subsequent scan of data checking the "Append spots to the current spot list" box. This will use all of the reflections resulting in better determination of the twin components.
3. Specify the **Neighbor Distance**s.
The neighbor Distance is the distance between spots in pixels. Specify the distance for the X, Y and Z axes. The default values of 7, 7, and 3 are sufficient for most samples.
4. Specify the size of spot to find in the **Spot Size** edit box.
The default value of 15 is sufficient for most samples.
5. Specify the **Peak Threshold,** analogous to I/sig in D*TREK Find Spots.
6. Click **Run** when satisfied with your selections.

Index Spots

To index spots,
1. Click **Index Spots** on the Flow Bar.

The **Index Spots** dialog will appear.
2. Specify the reflections by selecting the appropriate radio-button.
3. If desired, check the **Use Known Unit Cell** check box, then specify the unit cell values.
4. Make any desired changes in **Vector** and/or **Deviation.**
4. Click **Run** when satisfied with your settings.

Refine Cell

The **Refine Cell** feature refines the crystal, crystal goniometer, detector goniometer and source properties in order to reduce the differences between observed and calculated reflection centroids. *CrystalClear* can display the observed and calculated reflection centroids, so the progress and validity of
refinement can be judged.
To refine cells,
1. Click **Refine Cell** on the Flow Bar.
The **Refine** dialog will appear.

2. Click **Run**.

Save Twin

1. Click **Save Twin** to save the current component. Return to **Index Spots** to index the remaining reflections and repeat the above steps until you are satisfied that you have found all of the twin components.

Get Twin Relationship

When you are satisfied that you have found all of the twin components click the **Get Twin Relationship**
on the Flow Bar. This will print the rotation angle and the orientation matrix between all the components.

Predict Spots

To predict spots,
1. Click **Predict Spots** on the Flow Bar.
The **Predict** dialog will appear.

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2. Select the images to be processed.
You can either select the desired images from the **Image List**, or specify a single range of image sequence numbers in the **Sequence** edit box.
3. Specify the **Expected Spot Size** for the Z axis, in degrees, 0.9 should be used as a default value.
4. If desired, check the **All twins** check box.
5. If desired, check the **Alpha2 spots** check box.
6. Click **Run**.
If you are satisfied that you have a rotationally twinned sample, please contact Rigaku/MSC for the latest
command line version of the TwinSolve module and further instructions on integrating your sample.

Strategy

Strategy can be used to automatically generate a collection schedule so you don't have to. Results are written to the file `dtstrategy.log` and are readily displayed within *CrystalClear*.
To process **Strategy**,
1. Click **Strategy** on the flow bar.
The **Strategy** dialog will appear.

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2. In **Search Resolution** group box, make changes to setting by clicking **Set** button.
The **Set Resolution** dialog appears:
For assistance in using the **Set Resolution** *dialog, see page 119 in* Section 8 Additional Processing.
3. Click the Advanced tab.

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4. In **Speed/Accuracy** group box, make appropriate selections:

- Very Fast 0.3
- Fast 0.6
- Accurate 1.0
- Custom Set by user

5. If desired, make changes in **Result Limit** and/or **Search Rotation** group boxes.
6. If you wish to **Use Previous Reflections** , check the box. Select the **Previous Reflection** by using the down-arrow.
7. If you with to use defaults from other projects, click the **Defaults…** button.
The **Get Defaults** dialog appears.
8. If you wish to **Save**, click the **Save** button.
The **Default Manager** dialog appears.

- *For assistance using the* **Default Manager**, *see page 209 in* Appendix F: Defaults in CrystalClear.

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9. When all desired settings are selected, Click **Run**.

Integration

The **Integrate** function predicts the reflections which would appear on a range of images. This process
may produce several reflection files. These files are merged as part of the **Integrate** function.

Integrate with d*TREK (RAXIS or Mercury CCD)

Integrated reflections are written to the file `dtintegrate.ref` and are readily displayed within *CrystalClear*.

To integrate images,

1. Click the **Integrate Reflections** button on the Flow Bar.

The **Integrate Reflections** dialog will appear.

2. Specify the images to be integrated. To specify a sequence of images. Then select the desired images
in the **To Use** entry field.

The **Integrate Reflections** dialog allows the user to enter image numbers manually or select images numbers from a list. Right-click on the **To Use** entry field to view menu options.

To enter image numbers manually in the **To Use** entry field, be sure to use a dash (-) to separate consecutive image entries and use a comma (,) to separate non-consecutive images entries. *For example, you can enter images such as 2-5, 7, 9-12.* Before clicking the **Run** button to **Integrate**

Reflections , de-select (un-highlight) the **To Use** entry field to verify the selected image entries

Right-click an entry field for further menu options as follows:

View Images List Displays a list of image files

Select Scan Allows user to select images of a scan

Clear Scan Clears selected images of a scan

3. Set the desired **Resolution**. If you wish to change the default resolution, click **Set**. If you specify 0.0
for both the minimum and maximum values, all reflections on the detector are predicted and integrated. See *Set Resolution* on page 119of *Section 8 Additional Processing* for more information on the **Set Resolution** function.

Resolution sets the resolution range of reflections to predict and integrate. Remember that low resolution reflections may be blocked by the beam stop, while high resolution reflections may be limited by the detector swing or edges.

4. In the Box **Width** and **Height** fields, set the integration box size in pixels.

*Be sure to choose a **Box size** that completely encloses the Bragg reflection and allows for changing spot shape and shifting spot positions due to misalignment of the hardware and/or a slipping crystal. A typical box size will be 6 to 10 times the spot dimensions. The larger the values of **Width** and **Height,** the more memory* CrystalClear *will use. It is normal and OK if neighboring reflections intrude into this box ¾ this will be predicted and excluded, but it should not intrude by more than one-half through the image.*

5. In the **Padding** field, specify the number of images to include in a three-dimensional integration volume (a shoebox) both before and after the predicted rotation width of a Bragg peak.

***Padding** allows for (1) a shift of the predicted peak position, (2) a change in crystal mosaicity, and (3) background pixels before and after the Bragg peak that lie on the Ewald sphere. The larger the value of **Padding**, the more memory* CrystalClear *will use.*

6. Specify the **Images Per Batch**.

This value is the number of images that are treated as a batch. Refinement is done after every batch of images with the centroids of strong reflections found in the images. Reflections in the batch of images will all have the same Batch *field in the `dtintegrate.ref` and `dtprofit.ref` files.*

*The larger the value of **Images Per Batch**, the more memory* CrystalClear *will use. You may wish to strive to have 100-1000 reflections per batch, so for crystals with large unit cells, you may set **Images Per Batch** to 2 or 3, while for crystals with small unit cells, you may set **Images Per Batch** to 10-20.*

7. In the **Peak Radius** field, specify the **minimum** and **maximum** reflection radius to use.

This is a measure of the minimum radius of a reflection in pixels. Since spot shape is automatically determined, this minimum radius should be smaller than the actual spot, so that the algorithm can use it is as a seed from which to grow the spot shape. The maximum radius should be larger than the biggest peak but smaller than one-half the box size. The shape of weak reflections is determined from nearby strong reflections.

8. Specify a **Batch prefix** to use for batch IDs or names given to reflections in the output reflection

lists.

Use this option to distinctly label reflections from different scans and/or crystals. The prefix should not be longer than 4 characters. If no prefix is specified here, a batch prefix may be added to any reflection list at a later time

9. Click the **Advanced** tab.

10. In the **Profile Analysis** group box, select whether you want CrystalClear to automatically pick a profile size, use no profile size (None), or define your own profile size.

If you select **User-Defined**, specify the sizes of the transformed local Kabsch 3D profile in degrees.

*The **Size 1** value is the angular spread of a reflection in directions tangent to the Ewald sphere, while the **Size 2** value is the angular spread of a reflection in the direction perpendicular to the reciprocal lattice vector when in the diffraction condition. Good starting values are 0.5 * arctan (spot_size / crystal_to_detector_distance) and max(crystal_mosaicity/3, 2 * image_rotation_width). These are the same as the Kabsch XDS parameters DIVRAD and DIVBET. For either, if a value of 0 is used, then an appropriate value is calculated. For either, if a negative value is used, then profile analysis is not performed.*

11. Specify the maximum number of seconds to wait for a required image to appear before stopping in

the **Wait Limit** field.

The value of 0 means do not wait, so if an image cannot be found, integration will finish.

12. Select the **Refinement Macro** to be used.

The choices are:

- Crystal, then all detector
- Detector, then all crystal
- Low reso, then all reso
- Single Step Refine
- All

13. Select the **Pre-refinement** to be used.

The choices are:

- None
- First image
- First & Last
- First, Last & Middle
- 1st images of 3 batches

- All images of 5 batches

14. In the **Ice Rings** box, make desired entries in the **Min Resin** and **Max Resin** fields, if necessary. Click the **Add** button, the **Ice Ring** dialog will appear prompting the user to enter the **Min** and **Max** resolutions of the Ice Ring.

*Alternately**, Min** and **Max** resolutions can be entered by clicking and dragging on the displayed image. This method provides a visual representation of the* **Ice Ring***, as well as providing numerical values in the entry fields.*

15. Click **Run** to integrate reflections.

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Analyzing the Data

Once integration is completed, you may wish to analyze the data for purposes of evaluating and determining Laue symmetry, centricity, and spacegroup. Additionally, cell transformations and cell reduction tools are available here.

Click **Data Analysis** on the Flow Bar.

Several buttons become available.

Laue Symmetry

1. Click **Laue** on the flow bar.

The **Laue** dialog will appear.

2. Select the **Reflection List** file to use (generally dtprofit.ref).

3. Make other adjustments to settings as follows:

Max R-merge Tolerance for considering a Laue class present

Highest Laue Symmetry Limits the highest Laue class to be checked.

Only check Laue groups compatible with
current cell

Unchecked, examines all Laue classes
compatible with current cell

Average Bijvoets (Assume 1+ = 1-) Unchecked examines Laue classes desired

4. Click **Run**.

Centricity

1. Click **Centricity** on the Flow Bar.

The **Centricity** dialog will appear.

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2. Select the **Reflection List** file to use (generally dtprofit.ref).

3. Click **Run**.

4. Check the evaluation of centricity

Select the correct centricity if it is not already selected

5. Click **OK**

Spacegroup

1. Click **Spacegroup** on the Flow Bar.

The **Spacegroup** dialog will appear.

2. Select the **Reflection List** file to use.

3. Select the **<I/Sig>** value above which the reflections in the parity class will be considered present

Data Collection and Processing

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4. Click **Run**.

5. Carefully look through the table and evaluate if the **<I/Sig>** should be raised or lowered. Repeat the
run after you have made adjustments.

Scale and Average

The **Scale and Average** step calculates and applies scale factors to different batches of reflections in an
input reflection list, averages symmetry equivalent reflections, calculates merging and completeness statistics, and creates a reflection list of unique reflections.

Scale with d*TREK (RAXIS or Mercury CCD)

To Scale and Average your data,
1. Click the **Scale and Average** button on the Flow Bar.
The **Scale and Average** dialog will appear.
2. The **Reflection Lists** box displays the sample reflection list files. Select a reflection file.
3. In the **Algorithms** box, select the corrections to be applied. More than one may be applicable.

4. In the **Absorption Correction** group box, specify **Method** to use.

- Fourier
- Spherical 4,3
- Spherical 3,2

In order to perform an **Absorptive Correction**, the user must choose **Absorption Correction** from the **Algorithms** box (see Step 2).
If **None** is selected, specify **Max Cycles** also to perform Fox and Holmes scaling.
*If a method other than **None** is selected, the* REQAB *program of Dr. R. Jacobson is used to calculate and apply scale factors. The* REQAB *program usually gives the best results.*
5. Specify the number of **Max Cycles.**
This option refers to the maximum number of non-linear least squares cycles to perform. If the refinement converges, the maximum number of cycles may not be reached. No shifts are applied to the last cycle.
6. In the **Error Model** group box, specify a **Weight Multiplier** and **Weight Addend**.
7. Specify a value for **Exclude Sigma**.
*Input reflections with Intensity/sigma less than **Exclude sigma** are excluded from contributing to the scale factor refinement. However, these reflections are included in the final statistics and output files.*
8. Specify a value for **Rejection Sigma**.
*This field sets the rejection level for reflections measured more than once. Reflections with scaled intensities differing by more than **Rejection sigma** from the weighted average intensity calculated from other symmetry-related measurements are flagged as rejected by setting their observed standard deviations to be negative.*
9. If the user wishes, selection of rejected reflections may be based on **Chi^2** values (reflections above
set value of **Chi^2** are rejected) or **Max Fraction** values (only the worst reflections up to this fraction of total number of reflections are rejected.)
10. In **Scaled, Averaged Output File** , specify a name for the output file.
Click the **Advanced** tab to set advanced values.

11. Specify the desired Resolution.

If you wish to change the default resolution, click **Set**. See *Set Resolution* on page 119 of *Section 8 Additional Processing* for more information on the Set Resolution function.

12. Set the **Scaling Constraints**.

Batch ID: Specifies the name of the batch whose scale factors will remain fixed. The scale factors of all other batches will shift relative to this batch. Default: first batch in the input reflection list.

Scale Factor: Specifies the scale factor of the fixed batch. All shifted scale factors are rescaled, so this value remains fixed. Default: 1.

B-factor: *These options are only available when* ***None*** *is selected for the* ***Absorption Correction Method*** *list box on the* ***Main*** *tab.*

13. If you desire **Optional Output** file, click the appropriate option, then specify a name for the output
file in the **Output Name** edit field.

If set, the scaled, but unaveraged, reflections are written to the specified file. This may be useful for further scaling or for use with other averaging and rejection algorithms. Reflections rejected by the scaling process will have their `fSigmaI` *values set to 0 or less.*

Check the **Output hkl, I, SigI, No Header** check box if you want the output file to include only the h,k,l, Intensity and sigmaI fields in free format, with no header.

*Rejected measurements (sigmaI <= 0) will be excluded from this file. This format is suitable for input to many non-d*TREK programs such as teXsan for subsequent processing.*

14. When you are satisfied with your settings, click **Run** to run the **Scale and Average** step.

7 Tool Reference

CrystalClear provides tools for the following functions:

- Create, open, save and delete Proje cts and Samples
- View, edit and set *CrystalClear* state information
- Create new processing state
- Display scan state
- View instrument state display
- Manually control X-ray instrument
- Set user preferences
- View log files

Create a New Project and Sample

When a new **Login Name** and **Password** are used, the **New Project Wizard** assists the user in setting
up the first project and sample. A complete description of this process is available in *Section 4 Running*
CrystalClear for the First Time on page 27. Once the initial project is set up, additional projects and samples are created using the following procedure.

1. Start *CrystalClear* and log in.

The **Open Sample** dialog is displayed.

- *Alternatively, the Open Sample dialog can be accessed on the* CrystalClear *menu. Click* ***File > New Sample or New Project*** *to create a new project and sample.*

The project/sample listed in the entry field(s) is the project/sample most recently updated by the user.

Additional projects/samples can be viewed and/or selected by clicking the appropriate down arrow(s).
*If the **New Project Wizard** appears, rather than the **Open Sample** dialog, it means* CrystalClear *did not find an existing project database file. Follow the steps in* Section 4 Running CrystalClear for the First Time *on page 27 to set up the first project and sample, or see your administrator.*

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2. To create a new project, click the **New Project** radio button.
The existing project name will be highlighted.
3. Type the new project name in the **Project** edit field. This will replace the existing text.
4. Click and highlight the existing Sample name. Type the new sample name in the **Sample** edit field.
This will replace the existing text.
5. Select the task you wish to use for this sample from the **Task** drop down list.
6. Specify the directory with the images for this project. Type the full directory name in the **Image Directory** field. If image files already exist, select using the **Browse** button.
CrystalClear can be used to process data collected previously. Images collected with CrystalClear, or other software, should contain header information with common filename extensions. Images collected
with the Rigaku R-Axis detector use filename extension .OSC. Images collected with the Rigaku Mercury or Jupiter CCD detector use filename extension .IMG.
CrystalClear will support .IMG (CCD), .OSC (RAXIS), and .STL (RAXIS) image files.
CrystalClear
will also support Bruker, MAR CCD, MAR IP, ADSC CCD, MacScience, Brandeis CCD, and MedOptics image files.

Create a New Sample

Following the first Login to *CrystalClear*, at least one project and sample had been created in the user's
database.
To create additional samples,
1. Start *CrystalClear*. Enter your **Login Name** and **Password**.
The **Open Sample** dialog will appear. The names listed in the entry fields are the Project and Sample most recently updated by the user. Additional projects and samples can be viewed and/or selected by clicking the appropriate down arrow.

- *Alternatively, the Open Sample dialog can be accessed with the Toolbar icon .*
- *The Open Sample dialog can also be accessed from the* CrystalClear *menu. Click **File > New Sample** to create a new project sample.*
- *The Open Sample dialog can also be accessed with the shortcut (Ctrl+N).*

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2. Click the **New Sample** radio button. The existing sample name will be highlighted.
3. Type the new sample name in the **Sample** edit field. This will replace the existing text.
4. Select the desired project from the **Project** drop down field.
By default, the last project you worked on will automatically be selected.
5. Select the task you wish to use for this sample from the **Task** drop down list.
6. Specify the directory with the images for this project. Type the full directory name in the **Image Directory** field. If image files already exist, select using the **Browse** button.

Open an Existing Sample

Following the **Login** procedure for *CrystalClear*, the **Open Sample** dialog appears. The **Project** and **Sample** listed in the entry field are those most recently opened by the user. Other **Projects** and **Samples**
can be accessed by clicking the down arrows.

- *Alternatively, access the Open Sample dialog with the Toolbar icon .*
- *The Open Sample dialog can also be accessed with the shortcut, (Ctrl+O).*
- *The Open Sample dialog can also be accessed from the* CrystalClear *menu. Click* ***File > Open Sample*** *to open a sample.*

1. Following the **Login** procedure,
the **Open Sample** dialog will appear.

Tool Reference

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2. Select the desired project from the **Project** drop down list.
3. Select the desired sample from the **Sample** drop down list.
4. Click **OK**.

Close the Current Sample

When *CrystalClear* closes a sample, the changes made during that work session may be saved or discarded.

1. To close the current sample, click **File > Close Sample** .
The following CrystalClear dialog will appear,
This dialog allows the user to save changes made to a sample, or discard changes made during that session. Once the sample is closed, the user is free to open another sample or create a new project or sample.

Save the Current Sample

To save an open sample, click the **Save Sample** button on the Toolbar .
If a new sample is created when another sample is current, *CrystalClear* saves and closes the current sample. Upon exiting *CrystalClear*, the current sample is saved and closed.

Tool Reference

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- *Alternatively, access the save feature from the* CrystalCle ar *menu. Click* ***File > Save Sample*** *to save the current sample.*
- *The save feature can also be accessed with the* CrystalClear *shortcut, (Ctrl+S).*

Delete Projects and Samples

To delete a project or sample from the *CrystalClear* database,

1. Click **File > Delete Projects/Samples**.
If a current sample is open, the following CrystalClear dialog appears. If you wish to close the current sample and continue the delete procedure, click **Yes**.
The following CrystalClear *dialog appears. To continue with the delete procedure, read the warning and click* ***OK***.
The **Delete Projects/Samples** dialog will appear.

Tool Reference

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2. Select (highlight) the project or sample you wish to delete, then click the appropriate **Delete Project(s)** or **Dele te Sample(s)** button.
The project or sample will be removed from the CrystalClear *database. These files will also be removed from the actual files and directories where the project and sample files were stored.*
WARNING! Selecting a ***Project*** *will delete the Project and ALL Samples within that Project.*

Processing State - View, Edit and Set

The processing state is a collection of crystal and instrument parameters associated with each step of processing the data. A Processing State consists of default, calculated or refined crystal, detector, and source values. For example, a current sample is in one state following Index Spots and in a different state
following Refine Cell. The Processing State of the current sample can be viewed while processing the
data.

To view the **Processing State Display** window,

1. Click the **Show Processing State Display** toolbar button .

The **Processing State Display** window will appear.

- *Alternatively, access* **Processing State Display** *from the* CrystalClear *menu. Click* ***View*** **>** ***Processing State Display***.

Tool Reference

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The information in the **Processing State Display** *is as follows*:

Current State: The current processing state is displayed.

State History: Previous states are displayed in a drop down list. If desired, one may select a previous state and set it as the current state.

Scans: Click the down arrow to view a listing of scans

Crystal: Settings for the crystal can be viewed and changed. These are the same settings as in the **Setup**
dialog on the **Crystal1** and **Crystal2** tabs.

Spacegroup: Settings for the Spacegroup can be viewed and changed. These are the same settings in the **Setup** dialog on the **Crystal2** tab.

Detector: Settings for the detector are specific for the scan. Settings can be viewed and changed. These
settings are the same settings as in the **Setup** dialog, **Detector** tab. If the values in the **Scans** field are changed, the **Detector** settings may change.

Source: Settings for the X-ray source can be viewed and changed. These are the same settings as in the
Setup dialog on the **X-ray Source** tab.

The settings in the ***Processing State Display*** *are the same settings in the* ***Setup*** *dialog. The* ***Processing***

Tool Reference

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State Display *presents different view. This display is accessible during data processing.*

To change the current state,

1. Click the **State History** drop down list.

2. Select the desired state.

3. Check the values in all fields.

If correct, click the **Set As Current** button.

All parameters will be set to the values that were active during the selected state.

Create a New Processing State

You can create your own processing state, as well as selecting an existing state.

To create a custom state,

1. Click the **Show Processing State Display** toolbar button .

The **Processing State Display** dialog will appear.

- *Alternatively, access* **Processing State Display** *from the* CrystalClear *menu. Click* ***View > Processing State Display***.

Tool Reference

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2. Select the state that is most like the new state you wish to create from the **State History** drop down
list.

3. Change the desired parameters in the **Processing State Display** window.

Save Changes to New State or **Discard Changes**. *If you want to go back to the original settings, click the* **Discard Changes** *button.* **Discard Changes** *sets all the current parameters back to the values active during the previous state*.

4. Click **Save Changes To New State**.

The **New State** dialog will appear.

5. Type a name for your new state and click **OK**.

The **New State** *will automatically become the current state. The* **New State** *will be saved with the sample, along with all other states The* **New State** *will be placed in the* **State History** *list..*

Tool Reference

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View the Scan State Display

The **Scan State Display** shows all image information relevant to the current sample. All images and scans available for collection and processing can be viewed. The **Scan State Display** also allows the user to modify scans.

To view the **Scan State Display** window,

1. Click the **Show Scan State Display** button on the toolbar .

The **Scan State Display** window will appear. *CrystalClear* displays a window specific to the Image Collection Device Type selected; namely R-Axis, Jupiter CCD, or Mercury CCD.

- *Alternatively, click* ***View > Scan State Display*** *on the* CrystalClear *menu.*

The information reported on the **Scan State Display** is as follows:

Screen group box contains*:*

Schedules*:* Use the down-arrow to view additional **Schedules**. User may **Add**, **Delete**, or use **Manager** on **Screen Schedules.**

Scan Table: User may **Add Scan** or **Delete Scan** on the **Scan Table**, then make changes to scan settings, as desired.

For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.

Collect group box contains*:*

Schedules: Use the down-arrow to view additional **Schedules**. User may **Add**, **Delete**, or use **Manager** on **Collect Schedules.**

Scan Table: User may **Add Scan** or **Delete Scan** on the **Scan Table**, then make changes to scan settings, as desired**..**

For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.

Save: When Save is clicked, the **Default Manager** appears. *For assistance, see* **Using the Default Manager** *on page 209 of Appendix F: Defaults in CrystalClear.*

Sync with Disk: In a Process task, **Sync with Disk** updates the image directory on the drive and updates the **Scan State Display**. This is a valuable option if more images are available than when the sample was initially created.

If the R-Axis is the **Image Collect Device Type** , the following window will appear.

Tool Reference

CrystalClear User Manual Page 103

If Mercury CCD is the **Image Collection Device Type** , the following window will appear.

Using the Scan Table

The Scan Table is useful in changing various settings of scans in a Collect Schedule. The Scan Table consists of a series of manageable columns and column headings. The user can manipulate the Scan Table, allowing columns to be viewed or hidden, and columns widths can be changed. The Scan Table

Tool Reference

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is used to edit the various settings within a scan, to serve their particular needs within a Collect Schedule. Using the Scan Table consists of:

Manipulating the Scan Table: Assisting the user in viewing the **Scan Table** by clicking, dragging, and
viewing columns.

Editing the Scan Table: Assisting the user in altering the individual scan settings within the columns to achieve the desired **Collect Schedule** .

The **Scan Table** is accessible on the **Collect Images** dialog and on twice the **Scan State Display**.

- To access the **Collect Images** dialog: Click the **Collect Images** button on the Flow Bar during a **Collect** task.

(**Task** drop down list options: **Screen Collect and Process**, **Collect and Process**, or **Collect**.)

- To access the **Scan State Display**: Click the **Show Scan State Display** button on the toolbar.

Or, *click* ***View*** **>** ***Scan State Display*** *on the* CrystalClear *menu.*

The **Collect Images** *dialog and the* **Scan State Display** *window displayed in* **CrystalCle ar** *is specific to the Image Collect Device Type selected; namely, R-Axis, Jupiter CCD, or Mercury CCD. Even if your display is different from that illustrated in this manual, the instructions are the same.*

The following **Scan Table** appears on the **Collect Images** dialog, and twice on the **Scan State Display**:

The **Scan Table** contains the following column headings:

Scan ID: Scan identification number.

Template: Base name of the image.

Detector Distance(mm):Crystal to Detector distance.

2-Theta(deg): 2θ offset of the detector.

Max Resolution: Specify maximum resolution in degrees.

Wavelength(λ): Specify the wavelength of your X-ray source. The wavelength is based on the Element type. When you selected an Element, a valid wavelength will be selected automatically.

Tool Reference

CrystalClear User Manual Page 105

Phi(ϕ): Specify the position of the crystal goniometer in degrees.

Rotation Axis: Phi (ϕ). (Phi (ϕ) is normally used for the R-Axis.

Start Angle: The angle in degrees of the start position.

End Angle: The angle in degrees of the ending position.

Width: The width of one image, in degrees.

Step: The angular distance between the start angles of two consecutive images in the scan.
Number Images: The number of images to be collected in the scan
Completeness: The percent completeness of the data in that scan.
Start Number: The start number to assign to the first image of the scan.
Exp Time: Specify exposure time in minutes.
Total Images: Specify total number of images.
Images Collected: Images already collected, if any.
Images Scheduled: Images currently scheduled for collected during next collection run.
Scheduled Start Angle: The angle in degrees of the start position for currently scheduled images.
Scheduled End Angle: The angle in degrees of the ending position for currently scheduled images.

Manipulating the Scan Table

The **Scan Table** can be easily manipulated using the computer mouse. Right-click on the various column contents or the column headings, or click and drag columns.

- Right-click any column heading: **All Columns** menu appears. This allows the user to select, de-select individual columns to be displayed If all column headings are selected, all columns are displayed.
- Right-click **Schedule** heading**:** A **Schedule All/Clear All** menu appears, in addition to the **All Column**s menu.
- Click and drag heading lines Dragging a vertical column line allows the user to widen column widths to view a column heading. Making columns narrow allows the user to fit more columns into the viewing area. Dragging on horizontal lines expands depth of the table.

Tool Reference

- Right-click column entries: Depending upon the particular column entry, a useful popup menu appears:
  - **View Images** – Set All – Unset All
  - **Propogate** – Down – Up - All.
  - **Autoset**

Editing the Scan Table

Editing the **Scan Table** allows the user to change settings in various scans in a **Collect Schedule** . After using the **Add Scan** button, changes in column entries/values can be made.

1. When the **Add Scan** button is used, scans are added to the list.
*Each image is named by using the **Scan Template Name**, then adding on a numeric value. The number will increment by one with each added image, and is usually four digits long.*
A filename extension, such as .osc (for R-AXIS images) or .img (for CCD images) completes the filename. For example, for the **Project**-*Myoglobin and* **Sample**-*My, if the **Root Image Name** is Myo3, and the **Start #** is 1; then the image files will be named Myo30001.osc, Myo30002.osc ,Myo30003.osc., and so on. For Collect Sample, the Scan Template name defaults to the Sample name.*
2. Double-click in the **Start Angle** field to specify the starting angle for the scan.
Initially, this field may be set at 0.00 or set at the angle determined in the **Strategy** *step. However, if a scan should be stopped for some reason, the* **Start Angle** *should not be reset in order to continue*

the scan.
See Strategy *on page 80 of* Section 6 Data Collection and Processing *for assistance if necessary.*
3. Double-click in the **End Angle** field and specify the ending angle for the scan.
For example, if images are to be collected over the first 90 degrees of the sample, specify 90.0.
4. Double-click in the **Image Width** field and specify the width of an image in the scan.
Commonly the image width is 0.5 degrees.
5. Double-click in the **Exposure Time (min)** field and specify the length of time for the exposure. Units for the exposure time can be in minutes or seconds, depending on the procedure.
Refer to *General Settings* on page 141 of *Appendix B: Administration*. Additional information about changing the unit of exposure time is in *Set User Preferences* on page 110 of *Section 7 Tool Reference*
7. Double-click in the **Start #** field and specify the starting number for the images.
*The **# Images** and the **Completion Time** fields will be calculated automatically based on the values assigned in the various parameters.*

Tool Reference

CrystalClear User Manual Page 107
8. Make other adjustments to the settings as required.
For example, if you wish to scan 90° of the crystal with a 0.5° image width, and scan every 0.5°, your settings may be:
Start
Angle
End
Angle Width Step
#
Images
Completeness
Start
#
0.00 90.0 0.50 0.50 180 --- 1

View the Instrument State

You can view the state of the X-ray detector with the **Instrument State Display** window. The information reported is as follows:
To display the **Instrument State Display** window,
1. Click the **Show Instrument State Display** toolbar button.
- *Alternatively you can click **View > Instrument State Display** on the menu.*

The information reported on the **Instrument State Display** is as follows:
X-ray Source group box: Information about the X-ray **Shutter**, orientation, Source Type and **Optic Type** .
Goniometer group box: Information on the **Crystal** orientation and **Detector position**.
Detector group box: Information on **Image**, **Requested Settings**, **Expected finish time** , and **Detector type.**
The **Instrument State Display** window will appear. *CrystalClear* displays a window specific to the selected **Image Collection Device Type** ; namely R-Axis, Jupiter CCD or Mercury CCD.
If the R-Axis is the **Image Collect Device Type** , the following window will appears.

Tool Reference

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If Jupiter CCD or the Mercury CCD is the **Image Collection Device Type** , the following window will appear.

Manually Control the Detector

The instrument can be controlled from within *CrystalClear* with the **Manual Instrument Control** feature.

Items that can be controlled include:

- Goniometer and detector positioning
- Shutter control
- Imaging plate positioning and reading

Tool Reference

CrystalClear User Manual Page 109

- Complete instrument initialization
- Erase lamps illumination (R-Axis only)

To view the **Manual Instrument Control** window,

1. Click the **Show Manual Instrument Control** button on the Tool Bar .

- *Alternately, you can click **View > Manual Instrument Control** on the menu.*

The **Manual Instrument Control** dialog will appear. The options on the dialog will vary, depending on the detector that is currently selected.

If the R-Axis is the Image Collect Device Type, the following window will appear.

Tool Reference

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If the If Mercury CCD is the **Image Collection Device Type** , the following window will appear.

2. Select the desired setting and **Move!**

3. Click **Initialize** to datum the detector and goniometer.

Note: In general, one must initialize the instrument before running individual items.

Set User Preferences

Users can set preferences for how *CrystalClear* will appear on their computer screen. For example, a user may wish to turn off the message window, Command Bar and Status Bar to allow more space for
the image window.

Users can also specify their preferred language to be used within CrystalClear, where they want to store
certain files, whether to simulate the X-ray detector, and other user-specific preferences.

Select View Settings

To customize the **View Settings**,

1. Click **Tools > Preferences** on the menu.

The **Preferences** dialog will appear.

Tool Reference

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2. Check the desired options to appear on the *CrystalClear* interface.

3. Select the language to use in *CrystalClear*.

4. Continue to check other tabs or click **OK** to save changes.

Specify a directory for user files or scripts

To customize the locations of user files and scripts,

1. Click **Tools > Preferences** on the menu.

The **Preferences** dialog will appear.

2. Click the **Directories** tab.

Tool Reference

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3. Click the Ellipses Button to the right of the item you wish to modify.
The **Select Directory** dialog will appear.
4. Navigate to the directory to use, then click **OK**.
The selected directory will appear in the **Preferences** dialog.
5. Continue to check other tabs or click **OK** to save changes.

Specify Instrument Server Simulator

Tool Reference

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It may be limiting or unfeasible to run CrystalClear *only* on the computer connected to an Image Collect
Device (detector). For example, it may be necessary and convenient to process collected data on a computer other than the one connected to the Image Collection Device (detector); or it may be useful to
conduct in-house training sessions on *CrystalClear* on a computer other than that connected to the Image
Collection Device (detector).
CrystalClear provides an **X-ray Detector Simulator**. The detector simulator allows the processing of
data or user training on a computer other than the one connected to the Image Collection Device (X-ray
detector).
To configure *CrystalClear* to use the detector simulator,
1. Click **Tools > Preferences** on the menu.
The **Preferences** dialog will appear.
2. Click the **Server** tab.
3. In the **Run As Simulator** list box, check the box next to the name of the detector that you wish to run as a simulator.
4. Continue to check other tabs or click **OK** to save changes.

Configure the Instrument Server Simulator

Generally the instrument server simulators do not require changes to the configuration files. However,
note that the default images created by the server simulator will be “bogus”. Images created by the server simulator cannot be used for processing. The instrument server simulators should be reconfigured
to read previously collected images already on disk.

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When using the server simulator reconfigured to read previously collected images already on disk, all data collection conditions must be set up consistent with the parameters originally used in collecting the
images. (*i.e.*, scan rotation range, scan rotation axis, image width, direct beam position) in order to correctly process the images.

R-Axis Simulator

The R-Axis instrument server simulator, `MSCServDetRAXIS_Simulator.exe`, reads the same configuration file as its non-simulator counterpart, namely;
(`MSCServDetRAXIS.configuration`). The simulator interprets all options as the non-simulator

server, plus two additional options (which are ignored by the non-simulator server). These options are
SimulatorBaseFilename and *SimulatorMode*.
SimulatorBaseFilename = drive:\path\base
This option specifies the base name for the image files used by the simulator during data collection. The files should exist on the disk in the form *drive:\path\base???.img*, where *???* represents a number, padded on the right with 0s. All image numbers in a scan must have the same number of digits (*i.e.*, if there are 1000 images in the scan, then the first image number is denoted by 0001). In versions 2.1.2 and earlier, the minimum number of digits in the image number is three (3) (*i.e.*, image 1 is denoted by 001), unless the largest image number in the scan would require more than three (3) digits as described above. In versions 2.1.3 and later, the minimum number of digits in the image number is four (4).
SimulatorMode = realtime | immediate
This option indicates if the simulator will mimic real time when simulating exposures. If the value is *realtime*, then the exposures will take real time to finish (*e.g.*, a 30 second simulator exposure will take 30 seconds to finish). If the value is *immediate*, then the exposures will finish immediately.

CCD Simulator

The CCD instrument server simulators, namely; `MSCServDetCCD_Simulator.exe` and `MSCServCCDCamera_Simulator.exe`, read the same configuration files as the non-simulator counterparts (`MSCServDetCCD.configuration` and `MSCServCCDCamera.configuration`, respectively).). The simulators interpret all options as the
non-simulator servers, plus two additional options (which are ignored by the non-simulator servers). These options are *SimulatorBaseFilename* (MSCServCCDCamera) and *SimulatorMode* (MSCServDetCCD).
SimulatorBaseFilename = drive:\path\base
This option specifies the base name for the image files used by the simulator during data collection. This option is only recognized by the CCD Camera server simulator, `MSCServDetCCDCamera_Simulator.exe`. The files should exist on the disk in the form *drive:\path\base???.img*, where *???*

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represents a number, padded on the right with 0s. All image numbers in a scan must have the same number of digits (*i.e.*, if there are 1000 images in the scan, then the first image number is denoted by 0001). The previously collected images must be on a disk accessible by the framegrabber PC. The minimum number of digits in the image number depends on the version of `MSCServDetCCD_Simulator.exe`, not `MSCServCCDCamera_Simulator.exe`. In versions earlier than 3.0.0, the minimum number of digits in the image number is three (3) (*i.e.*, image 1 is denoted by 001), unless the largest image number in the scan would require more than three (3) digits as described above. In

versions 3.0.0 and later, the minimum number of digits in the image number is four (4), unless specified otherwise by the *MinimumScanTemplate* keyword in `MSCServDetCCD.configuration`.

SimulatorMode = realtime | immediate

This option indicates if the simulator will mimic real time when simulating exposures. If the value is *realtime*, then the exposures will take real time to finish (*e.g.*, a 30 second simulator exposure will take 30 seconds to finish). If the value is *immediate*, then the exposures will finish immediately.

Specify User Preferences

To customize other user preferences,

1. Click **Tools > Preferences** on the menu.

The **Preferences** dialog will appear.

2. Click the **General** tab.

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3. Select the **Scale and Average Graphs** to be displayed.

4. Set the **Resolution Units** for the image display

5. Set the **Exposure Time Units**, for data collection and image display.

6. Continue to check other tabs or click **OK** to save changes.

Specify Collection Defaults

To customize the preferences for setting up collection,

1. Click **Tools > Preferences** on the menu.

The **Preferences** dialog will appear.

2. Click the **Collection** tab.

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3. Make changes to the options.

4. Continue to check other tabs or click **OK** to save changes.

View Log Files

CrystalClear creates log files that help you "see" what settings were used during processing. The results
of the log files can help in troubleshooting problems.

To view a log file or another file in text mode,

1. Click the **View Log File** button on the Tool Bar .

The **Open** dialog will appear.

- *Alternatively, click **View > Log File** on the menu.*

2. Select the log file to view.
3. Click **Open**.

See *Appendix C: Sample Log Files* on page 161 for more information on log files.

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8 Additional Processing

Set Resolution

You can **Set Resolution** used during various data processing steps. Each of the following dialogs within
the processing procedure includes a **Set** button: Find Spots, Index Spots, Refine Cell, Predict Spots, Strategy, Integrate Reflections, Scale and Average. When this button is clicked, the **Set Resolution** dialog appears.
To **Set Resolution** for one or more processing steps,
1. Click the **Set** button on a displayed dialog displayed within processing procedure.
The **Set Resolution** dialog will appear.
2. Check the steps to set the default resolution.
3. Specify the resolution values in the **Minimum** and **Maximum** edit windows; or press **To Edge of Image** or **To Corner of Image** buttons.
4. Click **OK**.
Once the resolution is set for each step, the specified values will appear on the respective dialog.

Merge Reflection Lists with d*TREK

In addition to scale and average in the d*TREK processing module, reflection lists can be merged separately. The **Merge Reflections** task will also merge reflection list files with different columns or fields.
To **Merge Reflection Lists**,
1. Start *CrystalClear* and log in.
2. At the **Open Sample** dialog, select a sample.

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*This sample should have been processed at least up through **Integrate Reflections**.*
3. At the **Task** drop down list, select **Combine Reflections** .
4. Click **Merge** on the Flow Bar.
The **Merge Reflection Lists** dialog will appear.
5. Select the reflection lists to be merged in the Reflection Lists list box.
6. Specify a name for the resulting output file in the **Output Merged File** edit field.
7. Specify a **Zone Type**. The available options are:
None, H00, 0K0, 00L, HK0, H0L, 0KL
8. To restrict resolution, check the **Restrict Resolution** check box, then specify the **Minimum** and **Maximum** values.
9. To **Import Reflection File** , click the button.
The **Select Reflection File to Import** dialog appears,

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a. There are several ways to select a file to import:

- Click to browse for a file to import.
- Select a file to import by clicking on it.
- Type the **File name** to import in the entry field.
- Click **Files of type** down arrow to view files other than (*.ref.)

b. Click **Open** to import the file.
Note: When files are imported, the filename is added to the **Reflection List.** *If the imported file has a unique name, it is placed in the list with the same name. If the imported file has a duplicate filename, it is augmented as "import1(filename). Doing a second file with the same name augments that filename to "import2(filename). See the* **Merge Reflection Lists** *dialog above.*
10. When satisfied with your selections, click **Run**.

Create and Edit Macros

Once a group of settings has been selected, it is convenient to quickly apply those settings. A macro

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allows you to store a group of settings for crystal refinement; then select the macro to quickly apply those settings. *CrystalClear* offers several predefined macros.

- All
- Single Step refine
- Detector, then all crystal
- Crystal, then all detector
- Lo reso, then all reso

CrystalClear also allows you to create and edit custom macros.

Creating a Macro

To create a custom macro,

1. On the **Refine** dialog, click the **Advanced** button.

The **Macro Editor** dialog will appear.

- *The* **Refine** *dialog can be accessed by clicking the* **Refine Cell** *button on the Flow Bar during a* **Processing** *task. (***Task** *drop down list options:* **Process** *or* **Screen Collect and Process***) Click the* **Advanced** *button to access the* **Macro Editor** *dialog.*

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2. Click the **New Macro** button.

The **New Macro** dialog will appear.

3. Enter a unique name for the **New Macro**.

4. From the list of *CrystalClear* predefined macros, select a macro with values similar to those to be used in the **New Macro**, then click **OK**.

5. The **Macro Editor** dialog will appear with a step-by-step list of the selected macro. Customize the macro by altering the values of the predefined macro. Highlight a step and change the values to reflect those desired. Continue to highlight steps and make changes as desired.

Use the **New Step** button to access the **New Refine Step** dialog to add a new step to the macro.

Use **Remove Step** button to delete the macro step selected.

6. When the customized **New Macro** is satisfactory, click **Close**.

When you click **Close** on the **Macro Editor**, the customized steps and values are saved with the **New Macro** name. This **New Macro** is specific to the current sample.

7. When the **Refine** dialog appears, click **Save**.

The **Default Manager** dialog appears.

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Default Manager dialog allows the **New Macro** to be saved at the Site Level, User Level, Project Level, or Sample Level. Using **Default Manager** allows you to use the **New Macro** in other projects and samples.

8. Choose the level or destination of the macro and click **OK**.

Edit a Macro

To edit a macro,

1. On the **Refine** dialog, click the **Advanced** button.

The **Macro Editor** dialog will appear.

- *The* **Refine** *dialog can be accessed by clicking the* **Refine Cell** *button on the Flow Bar*

during a **Processing** *task. (***Task** *drop down list options:* **Process** *or* **Screen Collect and Process***) Click the* **Advanced** *button to access the* **Macro Editor** *dialog.*
2. Select the macro you wish to edit from the macro list.
3. Edit the macro by changing the values of the listed macro. Highlight a step and change the values to
reflect those desired. Continue to highlight steps and make changes as desired.
Use the **New Step** button to access the **New Refine Step** dialog to add a new step to the macro.

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Use **Remove Step** button to delete the selected macro step.
4. When all macro steps are satisfactory, click **Close**.
When you click **Close** on the **Macro Editor**, the customized steps and values of the edited macro are saved specific to the current sample.
5. When the **Refine** dialog appears, click **Save**. The **Default Manager** dialog appears. This dialog allows the edited macro to be saved at the Site Level, User Level, Project Level, or Sample Level.
6. The **Default Manager** allows you to use the edited macro in other projects and samples. If you wish
to use the edited macro on additional projects, or make it available to other samples or all projects, make the appropriate selections on the **Default Manager** dialog, then click **OK**.

The Collect Schedule

The **Collect Images** dialog is useful in working with **Collect Schedules.** New schedules can be created,
existing schedule can be imported and altered to meet the various needs of each user. The **Collect Images** dialog is used to Run and Save **Collect Schedules**.
Use the **Collect Images** dialog to:

- Create a Collect Schedule
- Import a Collect Schedule
- Run a Collect Schedule
- Save a Collect Schedule

1. Access the **Collect Images** dialog.

- *The* **Collect Images** *dialog can be accessed by clicking the* **Collect Images** *button on the Flow Bar during a* **Collect** *task. (***Task** *drop down list options:* **Screen Collect and Process**, **Collect and Process**, *or* **Colle ct**.*)*

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Note: When CrystalClear *is using the R-Axis as the Image Collect Device Type, the illustrated* **Collect Images** *dialog appears. When* CrystalClear *is using the Mercury CCD Image Collection Device Type, a slightly different* **Collect Images** *dialog appears. The following instructions apply for both dialogs.*

Create a Collect Schedule

To create a new collect schedule,
1. Access the **Collect Images** dialog.

- *The* **Collect Images** *dialog can be accessed by clicking the* **Collect Images** *button on the Flow Bar during a* **Collect** *task. (***Task** *drop down list options:* **Screen Collect and Process**, **Collect and Process**, *or* **Collect**.*)*

2. Use the **Scan Table** to alter the scans::

- *Use the* **Add Scan** *button to increase the number of scans at a different crystal orientation. Adjust settings as desired.*

- *Use the* **Remove Scan** *button to remove undesired scans.*

For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.

3. Make adjustments to the settings as required.

4. When all settings are satisfactory for the new **Collect Schedule,** you can:

- **Run** See *Run a Collect Schedule,* on page 128, for assistance.
- **Save** See *Save a Collect Schedule,* on page 127, for assistance.

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Import a Collect Schedule

To import an existing collect schedule,

2. Access the **Collect Images** dialog.

- *The* **Collect Images** *dialog can be accessed by clicking the* **Collect Images** *button on the Flow Bar during a* **Collect** *task. (***Task** *drop down list options:* **Screen Collect and Process**, **Collect and Process**, *or* **Collect**.*)*

3. Use the **Import** button to use an existing **Collect Schedule** from Project, User, or Site Levels.

- *If you wish to use the defaults of different Sample, you must open that Sample and Save the defaults at the Project, User, or Site level. For assistance, see* Using the Default Manager *on page 209 of* Appendix F: Defaults in CrystalClear.

The **Import Schedule** dialog will appear.

4. There are several options on the **Import Schedule** dialog:

- Use the **Rename** button to rename a selected schedule. A **Rename Schedule** dialog appears.
- Use the **Delete** button to delete a selected schedule. A **CrystalClear** warning dialog appears.
- Use the **Import** button to import a selected schedule. A **Name Schedule** dialog appears.

5. Use the **Close** button to close this dialog and return to the **Collect Images** dialog.

6. Manipulate the imported schedule, making changes to settings on the **Scan Table**, as desired.

For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.

Save a Collect Schedule

When the **Save** *button is used, the* **Default Manager** *dialog appears. For assistance using the* ***Default Manager Dialog****, see page 209 in* Appendix F: Defaults in CrystalClear, *for assistance.*

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1. When the **Collect Images** dialog **Save** button is clicked,
the **Default Manager** dialog will appear.

2. The **Default Manager** dialog allows the user to save the settings to various levels.
Select the **Current Levels** you wish to save by clicking the appropriate check-box.

- Alternatively, selections can be made by clicking the radio-button beside the appropriate Site, User, Project, or Sample names.

a. Use the following buttons for assistance in setting defaults:

- **Set** Sets a default
- **Unset** Unsets a default
- **Set All** Sets all Levels
- **Unset All** Unsets all Levels

Note: Only Users with Administrator privileges are authorized to set **Site** *Defaults. For most users, this option is grayed-out.*

Run a Collect Schedule

To run a collect schedule,
1. Access the **Collect Images** dialog.
- *The* **Collect Images** *dialog can be accessed by clicking the* **Collect Images** *button on the Flow Bar during a* **Collect** *task. (***Task** *drop down list options:* **Screen Collect and Process**, **Collect and Process**, *or* **Collect**.*)*

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2. Use the **Scan Table** to alter the scans, you may:
- *Use the* **Add Scan** *button to increase the number of scans at a different crystal orientation. Adjust settings as desired.*
- *Use the* **Remove Scan** *button to remove undesired scans.*

For assistance in manipulating the **Scan Table** *columns, headings or other settings, see* Using the Scan Table *on page 103 of* Section 7 Tool Reference.
3. Make adjustments to the settings as required.
4. When all settings are satisfactory for the new **Collect Schedule,** you can:
Click **Run** to start the scheduled collection.
The **Double-Check Settings** dialog will appear.
5. Review the specified settings on the detector.
6. Click **Start Image Collection**, or **Cancel Image Collection** if an error is found.
In the event CrystalClear detects insufficient disk space available for the entire data collection, a dialog will appear to guide you through selecting a new collection directory. You may need to "cancel" the data collection and free up space on the hard drive. If you wish to delete the images and processing from an old sample (presumably with all necessary file archived), see Delete Projects and Samples *on page 97 of* Section 7 Tool Reference

Delete Collection Schedule

To delete a collection schedule,
Access the **Scan State Display** dialog.

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Click the **Show Scan State Display** button on the toolbar .
Or click ***View > Scan State Display*** *on the* CrystalClear *menu.*
The **Scan State Display** window will appear. *CrystalClear* displays a window specific to the Image Collection Device Type selected; namely R-Axis or Mercury CCD.
1. Select the schedule in the **Collect Schedule** drop down box of the **Scan State Display** dialog.
2. Click **Delete** button.
3. Click **Yes** button to permanently delete the **Collect Schedule** .

Images

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9 Images

The Image Window

CrystalClear offers a graphical view of your data in the image window.
1 Large Image Window
2 Profile Windows
3 Large Image Window Toolbar
4 Small Image Window Toolbar
5 Small Image Window
6 Image Information Window

Large Image Window

The image is displayed in the large image window. Cross hairs allow you to select the portion of the image that will display in the Small Image Window.

Profile Windows

The profile windows display a graphical profile, showing you the values of the pixels that intersect the xand
y-axis cross hairs. To display the integrated intensity of a spot, click on the spot in the large image window. You can also click and drag across an area to see how the values change from pixel to pixel.

Images

Large Image Window Toolbar

You can manipulate the image in the large image window using the tools on the Image Window toolbar.

Select You can use the Select tool to point at a particular pixel and get information about that pixel in the Information Window. With the Select tool, you can also click to see a profile plot of pixel values in the Profile Window.

Magnify Choose the Magnify tool, then click in the image window to see a magnification of an area.

Zoom Choose this tool to zoom in or out.

To zoom in on a specific area: right-click, then drag out a box

To zoom in: left-click, then move the cursor up

To zoom out: left-click, then move the cursor down

Full View This tool returns the display back to full view after you have used the Zoom feature.

Pan This tool allows you to pan across the image. Choose this tool, then click and drag in the direction you wish to pan.

Measure This tool displays a measurement in angstroms between two points. Click on a point, then drag to a second point.

Profile Use this tool to get a profile of a cross section. Unlike the Select profile, which gives only right-angle profiles, with this tool you can get a profile of pixel values in a line connecting two points. Click on a point, then drag to a second point to display the profile.

Add Spots With this tool, you can click on a spot to add it to the reflection list.

Delete Spots With this tool, you can remove spots from the reflection list. The spot closest to where you click will be removed.

Measure Pixels Use this tool to measure pixels in the Image Window.

Quad Erasure This tool is used to define a four-sided area to be masked out during processing. This is handy to remove the beam stop shadow from an image. To use, click in four corners of the area to be removed. (*See* **Non-uniformity Type** *on page 54 in Section 6 Data Collection and Processing for help with Mask Files*.)

Circle Erasure This tool is used to define a circular area to be masked out during processing. To use, click the center of the circular area, then drag to the outside edge of the area. When the mouse button is released, the circular area will be defined. (*See* **Non-uniformity Type** *on page 54 in Section 6 Data Collection and Processing for help with Mask Files*.)

Free-hand Erasure This tool is not yet implemented.
Undo Last Erasure This tool will undo the last erasure. This tool only allows a single undo.
Write File Save an image file. This tool allows for saving an image that has been modified.
Write Mask File Click this tool to save a mask file. The mask file is an image file that includes any erasures you might have made. (See *Quad Erasure* and *Circle Erasure or See* **Non-uniformity Type** *on page54 in Section 6 Data Collection and Processing for help with Mask Files*..)
Contrast Use this tool to adjust the contrast of your image.
Reverse Use this tool to reverse the pixel values in your image.
Color Use this tool to toggle between gray scale and color display.
Toggle Square Root Display
This tool displays the image with each pixel value being converted to its square root. This gives more contrast to the image, truncating the strong pixels and raising the display of weak pixels.
Reset Local Contrast This tool sets the contrast of the displayed portion of the image. This is useful in zoomed areas where there is a smaller or greater difference in minimum and maximum pixel intensities than the current contrast values.
Load Reflection List This tool loads a reflection list into memory. You can then add or remove spots with the Add Spots and Delete Spots tool; then use Write Reflection list to save the edited reflection list.
Write Reflection List This tool saves the current reflection list with any additions or deletions.
Set Reflection Size This tool allows you to adjust the size of the circle drawn around each spot. Note that this circle is for display purposes only and does not reflect the integration area or background/peak separation.
Toggle Filtering This tool allows you to filter out spots that are not found in the current image. For example, a spot that appears in Image 10 may not intersect Image 1. This tool filters out all spots whose rotation range does not intersect the displayed image.
Previous Image This tool displays the previous image in the series. For example, if the current image is Img004.osc, clicking this tool will display Img003.osc.
Next Image This tool displays the next image in the series. For example, if the current image is Img004.osc, clicking this tool will display Img005.osc.

Overlay Images Displays an image created from a specified series of images. Each pixel in the resultant image is generated by using the maximum value occurring in the images for that pixel position. This is generally used to display the image that would result from a wider rotation/oscillation angle.

Underlay Images Displays an image created from a specified series of images. Each pixel in the resultant image is generated by using the minimum value occurring in the images for that pixel position. This is generally used for examining the background over wide rotation/oscillation angle or for examining the extent of a reflection across several images and rotation angle values.
Average Images Displays an image created from a specified series of images. Each pixel in the resultant image is generated by using the average value occurring in the images for that pixel position.
Tile Images Displays an image created from tiling a specified series of images.
Spots that appear with a red circle during Integration are rejected spots (the spots may be saturated, or otherwise invalid), while those spots that appear within a red circle during refinement are spots whose difference between observed and calculated positions the exceed rejection limits in x, y, or ϕ. Spots that appear with a green circle during refinement have been excluded from refinement, either because they fall outside the resolution limits, or the lie too close to the rotation axis, or they are below the $I/\sigma(I)$ cutoff.

Small Image Window Toolbar

The toolbar for the small image window includes tools similar to the Large Image Window toolbar. However, they act upon the small image window only.

Small Image Window

A smaller portion of the image appears in the Small Image Window. You can select the portion that will appear here by moving the cursor in the Large Image window and clicking the mouse.

Image Information Window

Information about the image appears in the Image Information window. Much of the data listed here is for information purposes. However, you can manipulate such things as the number of spots displayed with the controls listed here. If a scroll bar appears, you can scroll up and down to see additional items in the control. If the background for a field is white, then that field is editable. To enact a change to the window, but not a permanent change to the state, enter the desired value and press Tab.

Appendix A: Files and Directory Structure

Appendix A: Files and Directory Structure

The *CrystalClear* program ships with the files in the following lists. Your installation may not include all files, depending on the detector type that your copy of *CrystalClear* came with.

Installed Files

CrystalClear program files

CrystalClear.exe Executable program file
CoreCode11.dll Shared code program library
CoreRes11ENG.dll English language resource file

CoreHobject11.dll DLL for database functions
gzip.exe Decompression utility used to decompress image files
DundasUG.dll DLL for table controls
system.configuration System configuration file
xg_dll.dll DLL for x-ray generator control

Compute Servers

MSCServDetCCD_Simulator.exe CCD compute server simulator
MSCServDetCCD.exe CCD compute server
MSCServDetCCD.configuration CCD compute server configuration file
MSCServDetRAXIS_Simulator.exe RAXIS compute server simulator
MSCServDetRAXIS.exe RAXIS compute server
MSCServDetRAXIS.configuration RAXIS compute server configuration file
RAXIS_IV.configuration RAXIS IV configuration file
RAXIS_IV++.configuration RAXIS IV++ configuration file
MSCServProcDTREK.exe D*TREK compute server
MSCServProcPROCESS.exe PROCESS compute server
MSCServProcTwinSolve.exe TwinSolve compute server
AFC7_RCD2.configuration Configuration file for AFC7 goniometer/RCD2 controller
AFC8_RCD3.configuration Configuration file for AFC8 goniometer/RCD3 controller
MercuryDefault.header Default header file for Mercury CCD
Errors.xer Twinsolve errors list
Huber.xpa Twinsolve file
huhelp.xhe Twinsolve help file
spacegrp.xsg Twinsolve spacegroup file

Help Files

CrystalClear.chm Online help file for CrystalClear
CrystalClearDoc.pdf Online Manual for CrystalClear
CoreHelp.chm Online help file for CrystalClear
TwinSolve.chm Online help file for TwinSolve module
infolist.txt Readme file containing release notes and other info
hh.exe HTML help engine
hhctrl.ocx Help engine file
itircl.dll Help engine file

Appendix A: Files and Directory Structure Images

itss.dll Help engine file
popup.ocx Help engine file

OCX Components

FlowCtrl.ocx Flow Control OCX
RegFlowCtrl.bat Batch file for registering FlowCtrl.OCX
UnRegFlowCtrl.bat Batch file for un-registering FlowCtrl.OCX
Regsvr32.exe Program that registers OCX components

RAXWish Files

deisl1.isu
_isreg32.dll
blt80b1.dll
raxvideo.exe
raxwish.exe

shape.dat
shape.ico
aaa.log
shape001.ppm
shape002.ppm
shape003.ppm
shape004.ppm
tcl80.dll
tclpip80.dll
tif2rax.exe
tk80.dll
tix4180.dll
raxshape.ini
autoexec.bat
raxvideo.ini Initialization file for RAXVideo.exe

Crypto-Box files

Version.txt (Win95/98)
Cbn.vxd (Win95/98)
Install.bat (Win95/98)
Marx.reg (Win95/98)
Readme.txt (Win95/98)
Cbn.inf (Win95/98)
Register.bat (Win95/98)
Marxdev1.ini (WinNT)
Marxdev1.reg (WinNT)
Marxdev1.sys (WinNT)
Marxdev2.ini (WinNT)
Marxdev2.reg (WinNT)
Marxdev2.sys (WinNT)
Marxdev3.ini (WinNT)

Appendix A: Files and Directory Structure

Marxdev3.reg (WinNT)
Marxdev3.sys (WinNT)
Cbnvdd.dll (WinNT)
Install.bat (WinNT)
All_devs.reg (WinNT)
Msdos.bat (WinNT)
Readme.txt (WinNT)
Regini.exe (WinNT)
Register.bat (WinNT)

Additional Files

tcl80p2.exe Tcl installation program
ws295sdk.exe Windows Sockets installation (required for Windows 95)
uninst.isu Uninstallation file
MoveData.dll DLL for MoveCCData.exe
MoveCCData.exe Moves and converts older databases to new version,

Files Created by CrystalClear

CrystalClear creates settings and script files:
AdminDatabase.ho Administration database file. This file is located in the Administration directory. It stores information about groups, users, servers, tools, modules, and default preferences.
InstrumentName.ho Databases detector-specific for settings. There is a defaults database file for every detector supported by *CrystalClear* in DATA\SiteDefaults. These files contain the default settings for new users. The settings stored in this file and are transferred to the *CrystalClearUserDefaults.ho* file each time a new user is added. Please refer to the document entitled "Defaults in CrystalClear" for more information on detector inheritance.
SiteInfo.ho Database for detector settings. This file is located in the DATA directory.
CrystalClearProjects.ho This file is located in each User directory. It includes a list of all the projects created for that user. Each user has a unique CrystalClearProjects.ho file.
CrystalClearUserDefaults.ho This file is located in each User directory. It includes the user's own default settings.
CrystalClearProjectDefaults.ho This file is located in the *User/Project* directory. This file includes defaults used when a new sample is created.
CrystalClearSamples.ho This file is located in the *User/Project* directory. This file is included in each project directory. It holds settings for each sample.
***Samplename*.ho** This file is located in the *User/Project/Sample* directory. Each sample will have its own *Samplename*.ho file.

This file holds current settings for the sample.
SessionScript.scp *CrystalClear* records all actions that change the program state in this file throughout the *CrystalClear* session. When a new session is started, the previous SessionScript.scp file is saved to SessionScript.bak, and a new SessionScript.scp file is created.
SessionScript.bak This file is a backup of the previous session SessionScript.scp. Only one previous session is saved in the SessionScript.bak.
Dtfind.log This is a log of the activity during a Find operation.
Dtindex.log This is a log of the activity during an Index operation.
Additional log files are created specific to the current operation.

Directories

A subdirectory called Data is created off the *CrystalClear* program directory. This subdirectory will contain information about the users, projects, and samples that are processed with *CrystalClear*.
Program Directory The directory where the *CrystalClear* program and its peripheral files installed.
Administration The Administration database is stored in this directory.
Data Directory The directory where the data about users, projects, and samples is stored. The data directory is a subdirectory of the Program Directory.
(User) Each user has a directory where their project and sample data is stored. The Administrator directory is a user directory created for the Administrator.

(User/Project) All of a user's projects have a unique directory located under the user directory.
(User/Project/Sample) A project can contain any number of samples. The sample data is stored in a unique subdirectory under the Project to which it belongs.
Scripts A script directory is created for each user. This directory is used by default to store the SessionScript.scp and SessionScript.bak files, as well as any scripts that the user may record. Users can change their script directory in Preferences, if desired.
Twinsolve A directory called c:\huber is created to store files required by the TwinSolve module.
RAXWish A directory called c:\RAXWish is created to store files required by the RAXWish software.

Appendix A: Files and Directory Structure

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DirectBeamShots A directory called `DirectBeamShots` is created, located off of the CrystalClear program directory for storage of direct beam shot information.
ContinuousIPReadImages A directory called `ContinuousIPReadImages` is created, located off of the CrystalClear program directory for storage of continuous IP Read information.
PMTCheckImages A directory called `PMTCheckImages` is created, located off of the CrystalClear program directory for storage of PMT Check Image information.

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CrystalClear has a built-in mechanism for managing various projects and samples, based on the **Login Name**. Once *CrystalClear* is installed, the administrator should specify default settings for the detector, and set up an account for each user. In order to add accounts to *CrystalClear*, you will need to log into *CrystalClear* as administrator.

Administrator Login

To log in as Administrator,
1. Start *CrystalClear*.
The **Login** dialog will appear.
2. In the **Login Name** edit field, Enter *Administrator*.
3. Leave the **Password** edit field blank, and click **OK**.
CrystalClear *ships with an Administrator account automatically set up. By default, this Administrator acount has no password (blank). A new password for the Administrator account should be set by using the procedure to* Edit User Settings *on page145 of* Appendix B: Administration.
4. At the **Open Sample** dialog, click **Cancel** to close the dialog.

General Settings

The *CrystalClear* administrator can set general defaults within the program. All settings made by the

administrator become default settings for new users at their initial login.

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To set defaults, access the **Administration** dialog.

1. At the menu line, click **Tools > Administration**.

The **Administration** dialog will appear.

The settings include view options. Select the options you wish to be displayed.

Standard Tools: Toggle the display of the standard tools, such as Open, Save, View Log file, etc.

View Tools: Toggle the display of the View tools

Task List: Toggle the display of the task box

Flow Bar: Turn display of the Flow Bar on or off (initial default = on)

Command Line Bar: Turn display of the Command Line Bar on or off (initial default = on)

Message Bar: Turn display of the Message Bar on or off (initial default = on)

Script Tools: Toggle the display of the script tools (play, record, pause and stop)

Status Bar: Turn display of the Status Bar on or off (initial default = on)

A default language for *CrystalClear* can be selected with the Default Language option.

Default Language: Select the default language for the application.

Administration of Users

With the **Administration** dialog, the Administrator can access the **Users** tab to add users, edit user settings, and remove users.

Note: When a new **Login Name** *is created, the general settings defined by the administrator are applied*

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to the user's personal settings database. Each user can modify their own settings for their **Login Name**

once they have logged in.

Add a User

To add a user,

1. Access the **Administration** dialog by clicking **Tools > Administration**.

The **Administration** dialog will appear.

If you have logged in as a user without administration privileges, the Tools > Administration option is disabled. Log in as Administrator to access this option.

2. Click on the **Users** tab.

3. Click the **Add** button

The **User Settings** dialog will appear.

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4. Enter the user new name in the **Name** edit box.

For the user's convenience, the name you enter in this field could be the same as the user's Windows login name. By default, **CrystalClear** *displays the user's Windows login name in the initial* **CrystalClear** ***Login Name*** *field.*

5. Enter a meaningful description of the user in the **Description** edit box. This description can be the person's full name, their job title, or any other text that is meaningful in your work environment.

6. Enter the path to the user's preferred data directory in the **Data** filename edit box.

If you leave this field blank, CrystalClear *will automatically create a subdirectory for the user, and that path will be displayed in this edit window when you edit the user's settings in the future.*

For example, the default directory for the user name Jesplin would be *c:\Program Files\Rigaku*

MSC\CrystalClear\data\Jesplin, if f:\data\Jesplin were not used.
7. In the **Password** group box, enter a user password in both the **New** and **Confirm** edit fields.
The password is not case-sensitive.
8. Select the default language to be used for the user.
English is the default language. In the future, other languages may be added to CrystalClear.
9. In the **Member of (Groups)** group box, select the groups(s) to which the user should belong. The user will be a member of all groups with a check in the box.
10. Click **OK** to add the user.

Remove a User

To remove a user,
1. Access the **Administration** dialog by clicking **Tools > Administration**.
The **Administration** dialog will appear.
If you have logged in as a user without administration privileges, the Tools > Administration option is disabled. Log in as Administrator to access this option.

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2. Click on the **Users** tab.
4. Select the user to be removed from the user list.
5. Click **Remove**.
The following **CrystalClear** dialog appears.
When you remove a user, you also be given the option of deleting the user's data and data directory.
6. Click the appropriate response:

- **Yes** Remove user and all directories
- **No** Remove user but do not remove all directories

Edit User Settings

Use this feature to edit a user's password, description, data path, or assigned groups
To edit user settings,
1. Access the **Administration** dialog by clicking **Tools > Administration**.
The **Administration** dialog will appear.
If you have logged in as a user without administration privileges, the Tools > Administration option is disabled. Log in as Administrator to access this option.
2. Click on the **Users** tab.

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2. Select the user name or Administrator from the **Users** list, then click **Edit**.
The **User Settings** dialog will appear.
3. Make the desired changes in the settings.
It is recommended that the default (blank) Administrator password be changed to a specific password to protect against unauthorized changes in the CrystalClear settings.
To change a **Password**, *enter the* **New** *password. Re-enter the password in the* **Confirm** *field.*
4. Click **OK** to save the changes.

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The user's current data will not be moved to a new user path.

Administration of Groups

To help manage the privileges given to different users, assign users to **Groups**. *CrystalClear* ships with
two pre-defined **Groups**: *Administrators* and *Users*. By assigning a user to the pre-defined

Administrators Group, the user will have privileges to add, edit, or remove users, groups, tools, or servers.
To administer groups,
1. Access the **Administration** dialog by clicking **Tools > Administration**.
The **Administration** dialog will appear.
If you have logged in as a user without administration privileges, the Tools > Administration option is disabled. Log in as Administrator to access this option.
2. Click on the **Groups** tab.

Add a Group

To add a group and create groups that use combinations of **Administrative** and **Application Rights**.
1. Click the **Add** button.
The **Group Settings** dialog will appear.

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2. In the **Name** edit field, enter a name for the user group.
3. In the **Description** entry field, enter a description for the new group.
4. In the **Administrative Rights** list, select the rights you wish to grant to members of this group.
5. In the **Application Rights** list, if applicable, select the rights you wish to grant to members of this group.
6. Click **OK** to save the new group.
*Once you add a new group, it will appear in the **Members of (Groups)** list in the **User Settings** dialog.*

Remove a Group

To remove a group,
1. Select the group to be deleted in the group list.
2. Click **Remove**.
When you delete a group, any users who are currently a member of that group will lose the rights given to them by being a member of that group. All other groups will remain intact, and the user will still have any rights granted to them by other groups.

Edit Group Settings

To edit a groups' selected privileges,
1. Select the group to be edited in the group list.

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2. Click **Edit**.
3. Make the desired changes, then click **OK** to save the changes.

Administration of Tools

You can add software tools to *CrystalClear* with the **Tools** tab in the **Administration** dialog. When you
add a tool, a menu entry for that tool will be added to the **Tools** menu. This makes it easy to access your
software tools from within *CrystalClear*.
To administer tools,
1. Access the **Administration** dialog by clicking **Tools > Administration**.
The **Administration** dialog will appear.
If you have logged in as a user without administration privileges, the Tools > Administration option is disabled. Log in as Administrator to access this option.
2. Click on the **Tools** tab.

Add a Tool

You can add tools, such as a script that you have created to automate the processing of a sample, or an
executable program.
To add a tool,
1. Click the **Add** button.
The **Tool Settings** dialog will appear.

2. In the **Name** edit field, enter the name of the tool.
*This name will appear on the **Tools** tab, and in the **Tools** pull down menu.*
3. In the **Command** edit field, enter the command line of the tool.
4. In the **Arguments** edit field, enter any arguments that are required for correct operation of the tool.
5. In the **Initial** edit field, specify the directory that should be active when the tool application starts.
6. If you want to be prompted for arguments when the tool starts, check the **Prompt for Arguments** check box.
7. If you want the tool to run without having a window pop up on the screen, select the **Run Minimized** check box.
8. If the tool is a script, check the **Tool is a Script** check box.

Remove a Tool

To remove a tool,
1. Select the tool to be deleted in the tool list.
2. Click **Remove**.
The tool will be removed from the Tool list in CrystalClear *only. It will not be deleted from the hard drive.*

Edit Tool Settings

To edit a tool's settings,
1. Select the tool to be edited in the tools list.
2. Click **Edit**.
3. Make the desired changes, then click **OK** to save the changes.

Administration of Servers

A server is a software package that interfaces with *CrystalClear*. The purpose of the server is to perform
complex calculations, and pass the results back to *CrystalClear*. *CrystalClear* ships with two compute
servers: d*TREK and PROCESS, and two instrument server, CCD control and R-AXIS control. When
you install *CrystalClear*, the servers are installed and configured automatically.
You cannot remove the servers, nor can you add additional servers to CrystalClear *at this time. The items that appear in the Servers list may vary, depending on which detector you have, and which servers
shipped with your particular copy of* CrystalClear.
To administer servers,
1. Access the **Administration** dialog by clicking **Tools > Administration**.
The **Administration** dialog will appear.

If you have logged in as a user without administration privileges, the Tools > Administration option is disabled. Log in as Administrator to access this option.
2. Click on the **Servers** tab.

Edit Server Settings

To edit the settings of a server,
1. Select the server to be edited, and click the **Edit** button.
The **Server Settings** dialog will appear.

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3. Change the desired options, then click **OK** to save the changes.
Path: Specify the path where the server program is located. By default the servers are installed in the same directory as the *CrystalClear* program. You can change this path if you need to move the server to another location. For example: c:\program files\Rigaku MSC\CrystalClear\dtrek.exe
Arguments: Specify any argument that you wish to pass to the server upon its startup. By default, no startup options are specified.
Description: Specify a description of the server software. For example, CCD Controller Software.
Options : Generally, if the server software were running in the background all the time, you would check the **Stand Alone Server** check box. The application would then forgo an attempt to start the server software when it is needed. However, *CrystalClear* always opens and closes the servers as needed, so you should leave this option unchecked.
IP Address: By default, the server software will use the local machine for processing the data. This is specified by the default IP address of 127.0.0.1. If you wish the server software to use a different machine for processing, specify that machine's IP address here.
Port: The Port options allow you to select the port to be used for communication between the application and the server software. (This is not referring to a port such as the serial or parallel port; rather it is a software communication port.) By default, a port value and port range have already been specified for you, and in most cases you can use the default values. However, if you are running other software that is using the same port as one of the servers, you can adjust the port ID here.
Auto Generate: If you are not sure what port may be free, you can select the **AutoGenerate** check box
to allow *CrystalClear* to select a free port for you.

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Port Number: To specify a specific unique port value, you can enter a value here. Generally, the default port will work fine. You should only change this value if you are familiar with your system and software.
Range: If you select **Auto Generate**, you may want to also specify a port range from which to choose a port ID. You can do so in the **Range** edit fields.
*Note: At this time,*CrystalClear *does not support adding or removing servers.*

Specify Default Site-level Settings

After installing *CrystalClear*, you should set the default settings for your site. These settings will be inherited by all projects that are created later.
To set the default settings,
1. Start *CrystalClear* and log in as the *administrator*.
2. Close the sample by clicking **Close** in the **Open Sample** dialog.

3. Click the **Setup** button on the Flow Bar.
- *Alternatively, you can click **Sample > Setup** on the menu bar.*

4. Make adjustments to the settings on each tab, then click **Save**.
The **Default Manager** dialog will appear.

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5. Check the **Site** radio button, then click **OK**.
*If the **Site** radio button in the* **Current Levels** *group box is grayed out, you do not have administrator privileges. Exit* **CrystalClear** *and log in as an administrator, then repeat these steps.*
6. Continue through all of the dialogs available from the flow bar, repeating steps 4 and 5 for each dialog.
The settings will be saved to the *CrystalClear* Site Default database. All the settings in this database will
be inherited by each proje ct as it is created. Users can modify these setting for their own projects and samples.
For additional information about the options in the **Setup** dialog, see page 50 in *Section*6 Data Collection
and Processing.

Set Up Image Collection Device Type

CrystalClear operates with either a Rigaku R-Axis or a Rigaku Mercury or Jupiter CCD image collection device. After you install the *CrystalClear* software, you will need to select the device type in
order to control the instrument.

Select the Image Collection Device Type

To select the correct device type,
1. Start *CrystalClear* and log in as the *administrator*.
2. Close the sample by clicking **Cancel** or **OK** in the **Open Sample** dialog.

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3. Click **Utilities > Administrator Utilities**.
The **Administrator Utilities** dialog will appear.
4. From the **Image Collection Device Type** drop down list, select the appropriate device.
The current choices are R-AXIS II, R-AXIS IV, R-AXIS IV++, AFC7 Mercury, AFC8 Mercury, AFC9 Jupiter, and AFC9 Jupiter210.
5. If changes are made in **Administrator Utilities**, the following **CrystalClear** dialog appears.
Click **OK**
You must exit **CrystalClear** and *restart the program in order for the new* **Administrator Utilities** *settings to be embedded.*
If no changes are made, close the **Administrator Utilities** dialog by clicking the on the upperright of the dialog box.
6. If necessary, exit **CrystalClear** by clicking the on the upper-right of the screen.
- *Alternatively, you can click **File > Exit** on the menu bar.*

Determine Direct Beam Position

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In order to correctly process data that have been collected on the instrument, the position of the direct Xray
beam on the face of the detector at 20 equal to 0 must be determined. This procedure **must** be

performed after every filament change (on instruments using a rotating anode source) or after replacing
the X-ray tube (on instruments using a sealed tube source). Note that the procedure outlined below can
also be used to align the detector to the X-ray beam (see the appropriate hardware manual for instructions on how to perform this procedure).
Note for R-AXIS users: On the R-AXIS IV and R-AXIS IV++ systems, the imaging plates (IPs) are attached to a flexible stainless steel belt. When each IP is placed in the expose position, the IPs are not
placed in exactly the same position (there is generally a 1 to 4 pixel difference in the position), effectively resulting in a two (2) detector system. Failure to correct for this effect can cause problems during processing, due to drastic changes in the direct beam position between successive images. The instrument server uses the direct beam position information to shift the images read from one of the IPs
when they are written to disk, so that the direct beam position on images from both IPs coincide, effectively reducing the system back to a single detector system.
Warning: In order to protect the detector, the direct beam shall always be attenuated during direct beam shots.
To take a direct beam shot,
1. Start *CrystalClear* and log in as the *administrator*.
2. Close the sample by clicking **Cancel** or **OK** in the **Open Sample** dialog.
3. Click **Utilities > Administrator Utilities**.
The **Administrator Utilities** dialog will appear.
4. Remove the beam stop.
Remember to return the beam stop when direct beam shots are complete.
5. Specify the settings for **Direct beam shots**.
a. Set the **Number of shots** to at least 5 for the R-Axis detector. For the CCD, only one (1) direct beam shot will be taken regardless of the value entered.
b. For R-AXIS detectors, the detector should generally be initialized (so that the IPs are erased) before taking direct beam shots, and so **Initialize before direct beam shots** should be selected.
6. Click **Take!** to take direct beam shot(s).
When doing direct beam shots, you do not need to turn down the generator, but you must place some attenuation in the X-ray beam.
The images generated during direct beam shots are placed in the `DirectBeamShots` subdirectory of
the Program Directory. The direct beam utility generates a log file, called `DirectBeam.log`, which
contains output information concerning the position and shape of the direct beam for each shot taken. For R-AXIS detectors, there also a summary at the end of the log file containing the important results from the direct beam shots. The direct beam utility also generates a summary file, called `DirectBeamSummary.log`, which contains the summaries for all direct beam shots taken on the detector.

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A summary of the typical log file `DirectBeam.log` generated by the direct beam shot utility can be
found in *Appendix C: Sample Log Files* on page 161.
7. Replace beam stop when finished.

8. Close the **Administrator Utilities** by clicking the on the upper-right of the dialog box.

Check PMT (PhotoMultiplier Tube)

On R-AXIS systems, to check the photomultiplier tube,
1. Start *CrystalClear* and log in as the *administrator*.
2. Close the sample by clicking **Cancel** or **OK** in the **Open Sample** dialog.
3. Click **Utilities > Administrator Utilities**.
The **Administrator Utilities** dialog will appear.
4. Specify if the instrument should be initialized before checking the PMT, by either checking (initialize the instrument) or unchecking (do not initialize the instrument) the **Initialize R-AXIS** check box in the **Photo Multiplier Tube (PMT) check** group.
5. Click **Take!** to check the PMT.
On CCD systems, this check is not available.
6. Close the **Administrator Utilities** by clicking the on the upper-right of the dialog box.
For information on how to interpret the result, consult the appropriate instrument hardware manual.
The images generated during the PMT check is placed in the `PMTCheckImages` subdirectory of the
Program Directory. The PMT check utility generates a log file, called `PMTCheck.log`, which contains
output information concerning the average background, 3σ level and the number of pixels having a value
of 0 in the image. The PMT check utility also generates a summary file, called `PMTCheckSummary.log`, which contains the summaries for all PMT checks performed on the detector.
A summary of the typical log file `PMTCheck.log` generated by the PMT check utility can be found in
in *Appendix C: Sample Log Files* on page 161.

Continuously Reading an IP

On R-AXIS systems, the system can be set up to continuously read the IPs. This is mostly used as a diagnostic tool and will normally only be performed by a Rigaku/MSC service technician. To put the RAXIS
in continuous IP read mode,

1. Start *CrystalClear* and log in as the *administrator*.
2. Close the sample by clicking **Cancel** or **OK** in the **Open Sample** dialog.
3. Click **Utilities > Administrator Utilities**.
The **Administrator Utilitie s** dialog will appear.
4. Specify the setting for the **Continuous IP Read** mode.
a) Specify the number times to read the IPs in the **Number of cycles** field.
b) If the R-AXIS should be initialized before performing the test, select the **Initialize R-AXIS** check box.
c) Select the **Write images to same file** check box if the images are to be written to the same file on disk. If this check box is unselected, then each image will be written to a separate file on disk. Unless there is a need for saving the images read, writing the images to the same file on disk is the preferred mode of operation. Each image is approximately 18 Mb in size, and so writing the images to separate files can quickly fill up the disk (which may be the system disk).
d) If it is desired that the X-ray shutter open briefly (for approximately 1 second) before reading an

IP, select the **Open X-ray shutter during read** option.
*Unless there is a valid reason for selecting this option, we strongly suggest that you **unselect** this option for safety reasons.*
5. Click **Take!** to begin the continuous IP read.
On CCD systems, this feature is not available.
The images generated during the continuous IP read check is placed in the `ContinuousIPReadImages` subdirectory of the Program Directory. The continuous IP read check
utility generates a log file, called `ContinuousIPRead.log`, which contains output information indicating the success of failure of each of the IP reads. The continuous IP read check utility also generates a summary file, called `ContinuousIPReadSummary.log`, which contains the summaries
for all continuous IP read checks performed on the detector.
A summary of the typical log file `ContinuousIPRead.log` generated by the PMT check utility can
be found in *Appendix C: Sample Log Files* on page 161.

Appendix C: Sample Log Files

During processing, *CrystalClear* records information in log files. You can use these log files to double -
check that the correct parameters were used during processing, and to help you refine your settings. Below is a list of the logs files that are created by the d*TREK compute server.

For d*TREK

Process	**Log Filename**
Find Spots	dtfind.log
Refine Spots	dtrefine.log
Index Spots	dtindex.log
Predict Spots	dtpredictspots.log
Integrate Spots	dtintegrate.log
Scale and Merge	dtscalemerge.log
Merge Reflections	dtreflectionmerge.log
Strategy	dtstrategy.log

For PROCESS

Process	**Log Filename**
Peak Search	psearch.log
Index	index.log
Refine	refosc.log
Integrate	integ.log
Merge	merge.log
Scale	scale.log
Post Refine	post.log
Average	average.log

For TwinSolve

Process Log Filename

The log files are stored in the Sample directory.

You can view the log files during processing to follow the progress of the job.
To view a log file during a processing step,
1. Click **Windows > Log File Viewer**.
The selected log file will be displayed on the screen.
If you wish to view log files from previous processing steps,
1. Click **View > Log File** .
The Open dialog appears.
2. Select the log file to view.
3. Click **Open**.
The selected log file will be displayed on the screen.

Find Spots Log

A summary of a typical log file, which is produced by **Find Spots,** is listed below. The filename is `dtfind.log.`

```
1 dtfind: Copyright (c) 1996 Molecular Structure Corporation
2 ...
3 File /user4/jwp/DATA/NUCL4/nucl4001.osc successfully opened.
4 Find object listing:
5 Sigma: 0
6 Minimum: 2000
7 Circle lim: 950, 950, 0, 1343
8 Rect lim: 19, 1881, 19, 1881
9 Spot wind.: 30, 30
10 Peak filt.: 6
11 Back. tile: 237, 237
12 Pad: 3
13 Seq. num.: 1, 1
14 Image dim.: 1900, 1900
15 3D dump: 0
16 There were 554 preliminary reflections found in a 2D search.
```



```
17 Average peak 3sigma size in pixels:
18 7.99 by 6.69 pixels.
19 dtfind: There were 553 spots found.
20 dtfind: Spots written to dtfind.ref
21 DTREK_STATUS: 0
```

If the sequence range had included multiple contiguous images and the 2D method was not specified, then lines 17-18 in the output above would have also included the peak size in degrees:

```
17 Average peak 3sigma size in pixels and degrees:
18 11.82 by 9.87 pixels by 0.66 degrees.
```

If the box size is incorrectly chosen, reflection centroids may not be accurate and subsequent autoindexing and refinement will fail. If the crystal is slipping during data collection, it will have multiple orientations and subsequent steps will fail. If the crystal is twinned or cracked, reflection centroids may come from different crystal fragments with different orientations and subsequent steps will fail.
For the lowest residuals during refinement between observed and calculated reflection centroids, it is best to have spots from a narrow rotation range. For a better refinement of detector position and crystal
properties, it is better to have spots from a wider rotation range.

Index Spots Log

A summary of a typical log file called `dtindex.log` that is created during the Index Spots procedure,

is shown below:

```
1 dtindex: Copyright (c) 1996 Molecular Structure Corporation
2 ...
3 Reciprocal lengths of shortest difference vectors:
4 72.6744
5 60.6784
6 57.6331
7 50.2659
8 42.3718
9 Method: Direct space cosine Fourier transform
10 Out header: dtindex.head
11 Max cell: 68.0689
12 Num diffs: 50
13 Spacegroup: 0
14 Verbose: 1
15 Performing direct space cosine Fourier transform indexing ...
16 Suggested grid interval is: 1.5
17 Suggested max cell is: 112.5
18 Actual grid interval is: 1.5
19 Actual max cell is: 112.5
20 Start peak minimum: 0.924801
21 Used peak minimum: 0.924801
22 Number of peaks found: 4
23 Start peak minimum: 0.647361
24 Used peak minimum: 0.647361
25 Number of peaks found: 5
26 Least-squares fit of reduced primitive cell to 44 lattice characters
```



```
27 sorted on decreasing (highest to lowest) symmetry.
28 Only solutions with residuals <= 10.0 are listed.
29 ========================================================================
30 Soln LeastSq Spgrp Cent Bravais a b c
31 num residual num* type type alpha beta gamma
32 ========================================================================
33 4 3.789 75 P tetragonal 71.698 71.698 106.730
34 90.000 90.000 90.000
35
36 6 3.735 21 C orthorhombic 100.969 101.820 106.730
37 90.000 90.000 90.000
38
39 9 3.677 5 C monoclinic 100.969 101.820 106.730
40 90.000 90.335 90.000
41
42 10 1.130 16 P orthorhombic 69.244 74.070 106.730
43 90.000 90.000 90.000
44
45 11 0.638 3 P monoclinic 74.070 69.244 106.730
46 90.000 90.457 90.000
47
48 13 0.000 1 P triclinic 69.244 74.070 106.730
49 90.457 90.000 90.482
50
51 ========================================================================
52 *Suggested spacegroup number until systematic absences are examined.
53 Enter solution number of your choice: 10
54 Solution number 10 selected.
55 Unit cell parameters and orientation angles
56 ========================================================================
57 Integer a b c
58 Num residual alpha beta gamma Rot1 Rot2 Rot3
59 ========================================================================
```

```
60 1 0.044 69.241 74.081 106.637 155.782 30.261 102.479
61 89.463 90.013 89.579
62 2 0.044 69.241 74.081 106.637 -155.782 -30.261 -77.521
63 90.537 89.987 89.579
64 3 0.044 69.241 74.081 106.637 24.218 -30.261 -77.521
65 90.537 90.013 90.421
66 4 0.044 69.241 74.081 106.637 -24.218 30.261 102.479
67 89.463 89.987 90.421
68 ================================================================
69 Enter your choice: 1
70 Orientation angles choice 1 selected.
71 Crystal listing:
72 Unit cell lengths: 69.2409 74.0809 106.6370
73 Unit cell angles: 90.0000 90.0000 90.0000
74 Unit cell volume: 546986.750
75 Orientation angles: 155.7821 30.2615 102.4790
76 Mosaicity: 0.300
77 Description: unknown
78 Spacegroup number: 16
79 name: P222
80 Num. equiv. posns: 4
81 dtindex - Wrote header file dtindex.head
82 DTREK_STATUS: 0
```

Appendix C: Sample Log Files

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Lines 3-8 The reciprocal lengths in Ångstroms of the shortest reciprocal lattice difference vectors are listed. These often (***but not always!***) suggest the longest unit cell length. Sometimes the difference vector indicating the longest cell length is not available from the input reflection list. Sometimes a split, cracked or twinned crystal will give extraordinarily long lengths which is diagnostic of these conditions.

Lines 15-19 A direct space cosine Fourier map is calculated for a hemisphere volume with radius 112.5 Å and grid size 1.5 Å. If the maximum cell length of the crystal is larger than the `Actual max cell` (line 19), then it will be impossible to get an initial cell, so set **Max Cell Length** in the dialog and re-run. For small cell lengths, if the `Actual grid interval` (line 18) is too large, then it will be difficult to get a solution, set **Grid Size** in the dialog and re-run.

Line 20 An initial minimum peak height in the Fourier map is determined and listed. Since the origin of the Fourier map (point 0,0,0) is normalized to have a value of 1, a peak minimum of 0.9 or greater suggests that a solution to indexing will be found. Initial peak minimums below 0.9 suggest a problem such as incorrect grid size, incorrect spatial distortion, incorrect direct beam position, incorrect detector position, or a split, cracked, or twinned crystal.

Line 22 Four peaks were found with a height above the minimum and at least 3 were non-coplanar and define a 3-dimensional lattice. If at least 3 non-coplanar peaks were not found, the peak minimum would have been lowered by 5% and the Fourier map searched again. This will be repeated until a solution is found or the minimum peak height is 0.3.

Lines 23-25 Just in case, after 3 non-coplanar peaks are found the peak minimum is reduced to 70% of
the original value and the Fourier map is searched again.

Lines 26-51 The 3 non-coplanar peaks are used to determine a reduced primitive cell. This reduced primitive cell is then fit with a least-squares procedure (Anderson & Bernstein, 1988; Paciorek & Bonin, 1992) to the 44 lattice characters (Int. Tables Vol. A, pp. 746). The solutions with residuals less than or equal to 10 are listed in order of decreasing symmetry. Usually, residuals below 5 have been solutions. ***Any lattice symmetry must be***

ultimately confirmed by examining symmetry in the diffraction intensities!

Line 53 Since **User Chooses Solution** in the menu was set, the user is prompted to select a solution. Solution 10 was selected.

Lines 55-68 The orientation angles for the selected cell and lattice are displayed sorted on an `Integer residual`. Residuals greater than 0.10 are considered poor solutions and suggest a problem such as incorrect spatial distortion, incorrect direct beam position, incorrect detector position, or a split, cracked, or twinned crystal. In general, orientations with the same residual are equivalent.

Line 69 The user was prompted to select a solution, and number 1 was selected.

Lines 71-80 The crystal cell properties are listed. Note that indexing does not determine the crystal mosaicity, but nevertheless a default value is listed (line 76).

Line 90 The resulting unit cell properties is written to the output header file `dtindex.head` which can be used as input to the next step: Refine.

Refine Spots Log

A summary of a typical log file created by **Refine Spots**, called `dtrefine.log`, is shown below:

```
1 dtrefine: Copyright (c) 1996 Molecular Structure Corporation
2 Header of file dtindex.head successfully read.
3 ...
4 Crystal listing:
```



```
5 Unit cell lengths: 69.2409 74.0809 106.6370
6 Unit cell angles: 90.0000 90.0000 90.0000
7 Unit cell volume: 546986.812
8 Orientation angles: 155.7820 30.2610 102.4790
9 Mosaicity: 0.300
10 Description: unknown
11 Spacegroup number: 16
12 name: P222
13 Num. equiv. posns: 4
14 CRYSTAL_Goniometer listing:
15 Description: Eulerian 3-circle
16 Number of values: 3
17 Name Datum Current Units Vector
18 ================================================================
19 Omega 0.000 Unknown deg ( 1.000, 0.000, 0.000)
20 Chi 0.000 Unknown deg ( 0.000, 1.000, 0.000)
21 Phi 0.000 Unknown deg ( 1.000, 0.000, 0.000)
22 ================================================================
23 Source listing:
24 Single wavelength: 1.5418
25 Polarization: 0.5, 1, 0, 0
26 Intensity: 0
27 RX_Detector listing:
28 Pixel dimensions: 1900, 1900
29 Nominal size in mm: 193.23, 199.5
30 Description: RAXIS conversion
31 RX_Goniometer listing:
32 Description: UNKNOWN
33 Number of values: 6
34 Name Datum Current Units Vector
35 ================================================================
36 RotZ 0.000 Unknown deg ( 0.000, 0.000, 1.000)
37 RotX/Swing 0.000 Unknown deg ( -1.000, 0.000, 0.000)
38 RotY 0.000 Unknown deg ( 0.000, 1.000, 0.000)
39 TransX 0.000 Unknown mm ( 1.000, 0.000, 0.000)
40 TransY 0.000 Unknown mm ( 0.000, 1.000, 0.000)
```

```
41 TransZ/Dist 98.000 Unknown mm ( 0.000, 0.000, -1.000)
42 ================================================================
43 DetResolution min: 154180
44 DetResolution max: 1.6678
45 Refine resol min: 99999
46 Refine resol max: 1e-05
47 I/sigma cutoff: 0
48 Rejection limits: 1, 1, 2
49 Rel. rot. weight: 9999
50 Refinement results
51 ======================================================
52 Crystal
53 a, b, c: 68.6284 73.7186 106.5789
54 Sigmas: 0.0170 0.0102 0.0235
55 Shifts: 0.0000 0.0000 0.0000
```

Appendix C: Sample Log Files


```
56 alpha, beta, gamma: 90.0000 90.0000 90.0000
57 Sigmas: fixed fixed fixed
58 Shifts: fixed fixed fixed
59 Crys Rot1, Rot2, Rot3: 155.773 29.915 102.325
60 Sigmas: 0.0094 0.0029 0.0084
61 Shifts: 0.0000 0.0000 0.0000
62 Mosaicity: 0.300
63 Sigma: 0.0000
64 Shift: 0.0000
65 ======================================================
66 Detector: 0
67 Trans1, Trans2, Trans3: 0.074 0.069 97.871
68 Sigmas: 0.1201 0.1350 0.2432
69 Shifts: 0.0000 0.0000 0.0000
70 Det Rot1, Rot2, Rot3: 0.056 -0.026 -0.034
71 Sigmas: 0.1259 0.0640 0.0724
72 Shifts: 0.0017 0.0000 0.0000
73 ======================================================
74 Source
75 Wavelength, Rot1, Rot2: 1.5418 0.000 0.000
76 Sigmas: fixed fixed fixed
77 Shifts: fixed fixed fixed
78 ======================================================
79 Refinement residuals
80 rmsResid (mm) = 0.271192
81 rmsResid (Deg) = 0.292639
82 ======================================================
83 Reflections in list: 553
84 Reflections accepted: 514
85 Reflections rejected: 39
86 Reflections ignored: 0 (Outside I/sigI or Resolution limits)
87 dtrefine - Wrote header file dtrefine.head
88 DTREK_STATUS: 0
```

Lines 4-13 The original or starting crystal properties in the input header are listed.
Lines 14-22 The original crystal goniometer properties are listed.
Lines 23-26 The original source properties are listed.
Lines 27-42 The original or starting detector properties and position are listed.
Lines 43-44 The minimum and maximum resolution in Ångstroms of pixels on the detector are computed and listed.
Lines 45-49 The input (command line) options to Refine Spots are listed.
Lines 50-78 The refinement results (refined crystal, detector and source properties) are listed. The shifts shown are for the last cycle and should be very close to 0.0000. Any property not

refined will have the word "`fixed`" in the output or possibly `0.0000` for the estimated standard deviation.
Lines 79-82 The root-mean-square residuals for the observed reflection centroids in millimeters and degrees are shown. Residuals depend on spot centroid variances which depend on the size of the detector pixels, whether the reflection centroids are from 2D (single image) or 3D (multiple images) data, the detector calibration, the spot size, the crystal mosaicity, the image rotation angle increment, etc. For 2D data, the residuals will be higher than with 3D data. Typical values for 2D data when the image rotation width is less than the mosaicity are 0.1-0.4 mm and 0.1 to 0.5 degrees. For 3D data, these values are 0.05-0.1 mm and 0.05-0.1 degrees.
Lines 83-86 The number of input reflections is listed along with the number used in the refinement.

Those reflections that are rejected exceeded the rejection limits for the differences between observed and calculated centroid or were too close to the rotation axis. Those reflections that are ignored did not pass the Intensity/SigmaI and resolution limits.

Predict Log

```
1 dtpredict: Copyright (c) 1996 Molecular Structure Corporation
2 d*TREK version 6.1SSI -- Oct 27 2000
3 Command line:
4 dtpredict input.head -seq 180 180 -mosaicity 0.60 -out output.head -ref \
5 dtpredict.ref -display -list
6 Header of file input.head successfully read.
7 Crystal listing:
8 Unit cell lengths: 78.9495 78.9495 36.8831
9 Unit cell angles: 90.0000 90.0000 90.0000
10 Unit cell volume: 229893.231
11 Orientation angles: 58.4917 -54.9206 -90.2980
12 Mosaicity: 0.600
13 Description: unknown
14 RX_NONUNF_TYPE: >>None<<
15 Predict listing:
16 Spacegroup number: 96
17 name: P43212
18 Num. equiv. posns: 8
19 Equival. position 1:
20 1, 0, 0 0
21 0, 1, 0 0
22 0, 0, 1 0
23 Equival. position 2:
24 -1, 0, 0 0
25 0, -1, 0 0
26 0, 0, 1 0.5
27 Equival. position 3:
28 0, 1, 0 0.5
29 -1, 0, 0 0.5
30 0, 0, 1 0.75
31 Equival. position 4:
32 0, -1, 0 0.5
33 1, 0, 0 0.5
34 0, 0, 1 0.25
35 Equival. position 5:
36 0, 1, 0 0
37 1, 0, 0 0
38 0, 0, -1 0
39 Equival. position 6:
40 0, -1, 0 0
```

```
41 -1, 0, 0 0
42 0, 0, -1 0.5
43 Equival. position 7:
44 -1, 0, 0 0.5
45 0, 1, 0 0.5
46 0, 0, -1 0.75
```

Appendix C: Sample Log Files


```
47 Equival. position 8:
48 1, 0, 0 0.5
49 0, -1, 0 0.5
50 0, 0, -1 0.25
51 Crystal Orientation Matrix is:
52 [0][*]: -3.78606e-005, -0.00727938, 0.0103656
53 [1][*]: 0.00666557, 0.00880277, 0.00620622
54 [2][*]: -0.0230547, 0.0117159, 0.00814348
55 CRYSTAL_ Goniometer listing:
56 Description: Eulerian 3-circle
57 Number of values: 3
58 Name Datum Current Units Vector
59 ========================================================================
60 VirtualOmega 0.000 Unknown deg ( 1.000, 0.000, 0.000)
61 VirtualChi 0.000 Unknown deg ( 0.000, 0.000, 1.000)
62 Phi 0.000 Unknown deg ( 1.000, 0.000, 0.000)
========================================================================
63 Source listing:
64 Single wavelength: 1.5418
65 Direction vector: 0, 0, 1
66 Spectral Dispersion: 0.0002, 0.0002
67 Crossfire: 0.0002, 0.0002, 0, 0
68 Polarization: 0.5, 1, 0, 0
69 Size: 0, 0, 0, 0
70 Intensity: 0
71 RX_Detector listing:
72 Pixel dimensions: 3000, 3000
73 Nominal size in mm: 300, 300
74 Description: RAXIS conversion
75 Fast pixel vector: 1, 0, 0
76 Slow pixel vector: 0, 1, 0
77 Spatial distortion descriptive text:
78 Simple pixel scaling spatial distortion
79 Simple spatial distortion:
80 Center of primary beam: 1479, 1529
81 Pixel size (mm): 0.1, 0.1
82 Direction vectors: 0, 1, -1, 0
83 RX_ Goniometer listing:
84 Description: UNKNOWN
85 Number of values: 6
86 Name Datum Current Units Vector
========================================================================
87 RotAboutBeam 0.169 Unknown deg ( 0.000, 0.000, 1.000)
88 2Theta 0.079 Unknown deg ( -1.000, 0.000, 0.000)
89 RotY 0.214 Unknown deg ( 0.000, 1.000, 0.000)
90 XShift -0.054 Unknown mm ( 1.000, 0.000, 0.000)
91 YShift 0.120 Unknown mm ( 0.000, 1.000, 0.000)
92 Distance 119.478 Unknown mm ( 0.000, 0.000, -1.000)
========================================================================
93 DetResolution min: 154180
94 DetResolution max: 1.51956
95 DetResolution edge: 1.76436
96 Rotation list:
97 Start: 184.500
```

```
98 End: 185.000
99 Increment: 0.500
100 Time: 180.000
101 Oscillations: 0
102 Axis vector: 1, 0, 0
103 Axis name: Phi
104 Dark start: 0
105 Dark update: 0
106 Dark change limit: 0
107 DCoffset start: 0
108 DCoffset update: 0
109 Predict resol min: 999999
110 Predict resol max: 0.5
111 Component 1 crystal mosaicity: 0.6
112 dtpredict: There were 1339 reflections predicted.
113 Number of reflections written: 1339
114 dtpredict: Reflections written to dtpredict.ref
```

Strategy Log

```
1 dtstrategy: Copyright (c) 1997 Molecular Structure Corporation
2 d*TREK version 6.1SSI -- Oct 6 2000
3 Command line:
4 dtstrategy input.head -cmin 99.00 -rangemax 360.00 -lscale 0.30 -out \
5 output.head
6 Header of file input.head successfully read.
7 RX_NONUNF_TYPE: >>None<<
8 Setting predict resolution to detector EDGE, not corner!
9 Predicting reflections ...
10 Component 1 crystal mosaicity: 0.6
11 ... done. 8936 reflections predicted.
12 Crystal listing:
13 Unit cell lengths: 78.8782 78.8782 36.8650
14 Unit cell angles: 90.0000 90.0000 90.0000
15 Unit cell volume: 229365.567
16 Orientation angles: -53.5160 71.4165 -86.2778
17 Mosaicity: 0.600
18 Description: unknown
19 Spacegroup number: 75
20 name: P4
21 Num. equiv. posns: 4
22 Reducing reflnlist to asymmetric unit and sorting ...
23 ... done.
24 Searching for best rotation start and range ...
25 ... done.
26 Strategy results
==============================
27 Resolution: 23.66 - 1.76
28 Rotation start: 42.00
29 Rotation end: 102.00
30 Rotation range: 60.00
==============================
31 Completeness vs Rotation range
-----------------------------------
32 Rotation Cumul %Comp %Comp
33 range range shell cumul
-----------------------------------
34 42.0 - 47.0 5.0 15.1 15.1
```


```
35 47.0 - 52.0 10.0 15.4 31.9
36 52.0 - 57.0 15.0 16.3 45.9
37 57.0 - 62.0 20.0 14.4 58.4
```

```
38 62.0 - 67.0 25.0 15.0 69.7
39 67.0 - 72.0 30.0 15.6 77.7
40 72.0 - 77.0 35.0 14.5 85.1
41 77.0 - 82.0 40.0 15.6 91.4
42 82.0 - 87.0 45.0 14.7 94.5
43 87.0 - 92.0 50.0 15.4 97.1
44 92.0 - 97.0 55.0 13.8 98.5
45 97.0 - 102.0 60.0 15.0 99.1
-----------------------------------
46 42.0 - 102.0 60.0 99.1 99.1
47 Expected Completeness vs Resolution
-------------------------------------------------------------------------------
48 Resolution Calc Num Num Num Num Num Avg %Comp %Comp
49 range unique reflns rejs mults single unique mult shell cumul
-------------------------------------------------------------------------------
50 23.66 - 3.78 2777 5666 0 2037 592 2629 2.38 94.7 94.7
51 3.78 - 3.01 2592 5555 0 1888 703 2591 2.42 100.0 97.2
52 3.01 - 2.63 2370 5370 0 1925 444 2369 2.45 100.0 98.1
53 2.63 - 2.39 2481 5296 0 1814 666 2480 2.40 100.0 98.5
54 2.39 - 2.22 2370 5333 0 1814 555 2369 2.49 100.0 98.8
55 2.22 - 2.09 2666 6185 0 2222 444 2666 2.49 100.0 99.0
56 2.09 - 1.98 2370 5148 0 1814 555 2369 2.41 100.0 99.1
57 1.98 - 1.89 2481 5259 0 1888 592 2480 2.36 100.0 99.2
58 1.89 - 1.82 2185 5037 0 1666 518 2184 2.54 100.0 99.3
59 1.82 - 1.76 2629 5259 0 1777 777 2554 2.36 97.1 99.1
-------------------------------------------------------------------------------
60 23.66 - 1.76 24921 54108 0 18845 5846 24691 2.43 99.1 99.1
61 *** Note: cell length factor was 0.30, so the results above are approximate. ***
```

Integrate Log

An edited summary of a typical log file called `dtintegrate.log` that is created is shown following:

```
1 dtintegrate: Copyright (c) 1996 Molecular Structure Corporation
2 Header of file dtrefine.head successfully read.
3 RX_NONUNF_TYPE: >>None<<
456
Command line string: >>-reso<<
7 Command line string: >>-window<<
8 Command line string: >>-pad<<
9 Command line string: >>-profsize<<
10 Command line string: >>-batch<<
11 Command line string: >>-display<<
12 Command line string: >>-seq<<
13
14 ================================================
15 Integrate object listing:
16 ================================================
17 Verbose level: 1
18 Scan sequence range: 1, 20
19 Resolution range: 100, 3
20 Images/batch: 5
21 Batch prefix:
22 Image padding: 2
23 Window size: 30, 30
24 Profile size: 0.5, 0.5
25 ================================================
26
```



```
27 dtintegrate: 3D method used
28 RX_NONUNF_TYPE: >>None<<
29
30 File /user4//DATA/NUCL4/nucl4001.osc successfully opened.
31
```

```
32 ================================================================
33 ================================================================
34 IMAGE #: 1 (of 20)
35 Name: /user4//DATA/NUCL4/nucl4001.osc
36 Date: 25-Sep-1997
37 Time: 14:53:12
38 ================================================================
39
40 Rotation list:
41 Start: 24.000
42 End: 24.250
43 Increment: 0.250
44 Time: 120.000
45
46 Reflection dispositions
47 ================================================
48 Status: New Active Full DNormal DSpecial
49 Number: 340 340 0 0 0
50 ================================================
51
52 Shoebox dispositions
53 ============================================
54 Status: Total Filling Full Freed
55 Number: 1951 340 0 1611
56 ============================================
57
58 ...
59 File /user4//DATA/NUCL4/nucl4020.osc successfully opened.
60
61 ================================================================
62 ================================================================
63 IMAGE #: 20 (of 20)
64 Name: /user4//DATA/NUCL4/nucl4020.osc
65 Date: 25-Sep-1997
66 Time: 14:58:28
67 ================================================================
68
69 Rotation list:
70 Start: 28.750
71 End: 29.000
72 Increment: 0.250
73 Time: 120.000
74
75 Reflection dispositions
76 ================================================
77 Status: New Active Full DNormal DSpecial
78 Number: 0 338 338 648 90
79 ================================================
80
81 Shoebox dispositions
82 ============================================
83 Status: Total Filling Full Freed
84 Number: 1951 0 738 1213
85 ============================================
86 Refinement options found:
87 +CrysAll +DetAll -rej 1.0 1.0 2.0 -cycles 10 -weight 9999 -display -go
88 Refine listing:
89
90 Crystal listing:
91
```



```
92 Unit cell lengths: 68.7533 73.7744 107.0866
```

```
Unit cell angles: 90.0000 90.0000 90.0000
Unit cell volume: 543168.687
Orientation angles: 155.9357 29.9512 102.4337
Mosaicity: 0.480
Description: unknown

Spacegroup number: 16
name: P222
Num. equiv. posns: 4

CRYSTAL_Goniometer listing:

Description: Eulerian 3-circle
Number of values: 3

Name Datum Current Units Vector
=====================================================================
Omega 0.000 Unknown deg ( 1.000, 0.000, 0.000)
Chi 0.000 Unknown deg ( 0.000, 1.000, 0.000)
Phi 0.000 Unknown deg ( 1.000, 0.000, 0.000)
=====================================================================

Source listing:

Single wavelength: 1.5418
Polarization: 0.5, 1, 0, 0
Intensity: 0

RX_Detector listing:

Pixel dimensions: 1900, 1900
Nominal size in mm: 193.23, 199.5
Description: RAXIS conversion

RX_Goniometer listing:

Description: UNKNOWN
Number of values: 6

Name Datum Current Units Vector
=====================================================================
RotZ 0.230 Unknown deg ( 0.000, 0.000, 1.000)
RotX/Swing -0.026 Unknown deg ( -1.000, 0.000, 0.000)
RotY -0.042 Unknown deg ( 0.000, 1.000, 0.000)
TransX 0.092 Unknown mm ( 1.000, 0.000, 0.000)
TransY 0.061 Unknown mm ( 0.000, 1.000, 0.000)
TransZ/Dist 98.013 Unknown mm ( 0.000, 0.000, -1.000)
=====================================================================
DetResolution min: 154180
DetResolution max: 1.66982

Refine resol min: 99999
Refine resol max: 1e-05
I/sigma cutoff: 0
Rejection limits: 1, 1, 2
Rel. rot. weight: 9999

Refinement results
=====================================================
Crystal
a, b, c: 68.7510 73.7993 107.0777
Sigmas: 0.0032 0.0025 0.0053
Shifts: 0.0000 0.0000 0.0000

```

```
157 alpha, beta, gamma: 90.0000 90.0000 90.0000
158 Sigmas: fixed fixed fixed
159 Shifts: fixed fixed fixed
160
161 Crys Rot1, Rot2, Rot3: 155.938 29.965 102.437
162 Sigmas: 0.0012 0.0011 0.0035
163 Shifts: 0.0000 0.0000 0.0000
164
165 Mosaicity: 0.442
166 Sigma: 0.0221
167 Shift: 0.0000
168 ======================================================
169 Detector: 0
170 Trans1, Trans2, Trans3: 0.095 0.058 98.009
171 Sigmas: 0.0185 0.0138 0.0358
172 Shifts: 0.0000 0.0000 0.0000
173
174 Det Rot1, Rot2, Rot3: 0.252 -0.024 -0.043
175 Sigmas: 0.0166 0.0082 0.0085
176 Shifts: 0.0002 0.0000 0.0000
177 ======================================================
178 Source
179 Wavelength, Rot1, Rot2: 1.5418 0.000 0.000
180 Sigmas: fixed fixed fixed
181 Shifts: fixed fixed fixed
182 ======================================================
183 Refinement residuals
184 rmsResid (mm) = 0.0724333
185 rmsResid (Deg) = 0.0393826
186 ======================================================
187
188 Reflections in list: 648
189 Reflections accepted: 645
190 Reflections rejected: 3
191 Reflections ignored: 0 (Outside I/sigI or Resolution limits)
192
193
194 Strong peak info listing
195 ================================================================================
196 Area Num Intensity Sigma BackAvg BackSig Siz0 Siz1 Siz2 Dl Shft0 Shft1 Shft2
197 ================================================================================
198 1 0 0 0 0 0 0.0 0.0 0.0 0 0.0 0.0 0.0
199 2 8 824481 1482 705 84 13.0 12.6 3.0 11 -0.9 0.1 0.0
200 3 22 1667487 2064 831 92 12.7 14.5 4.8 12 0.1 0.0 0.0
201 4 21 1296592 1936 854 89 13.2 13.5 5.9 12 -0.5 0.3 0.0
202 5 15 578864 1376 774 84 12.9 11.8 3.1 9 0.0 0.6 0.0
203 6 0 0 0 0 0 0.0 0.0 0.0 0 0.0 0.0 0.0
204 7 0 0 0 0 0 0.0 0.0 0.0 0 0.0 0.0 0.0
205 8 133 783169 1433 820 88 14.4 10.2 2.8 12 -0.5 0.5 0.0
206 9 116 871217 1401 693 79 13.3 10.8 3.3 14 0.7 0.0 0.0
207 10 101 802518 1323 715 74 13.3 10.7 3.5 13 -0.3 -0.3 0.0
208 11 150 664956 1398 842 87 14.8 10.2 2.9 13 0.1 0.0 0.0
209 12 0 0 0 0 0 0.0 0.0 0.0 0 0.0 0.0 0.0
210 13 0 0 0 0 0 0.0 0.0 0.0 0 0.0 0.0 0.0
211 14 6 1027184 1709 698 83 13.0 13.2 3.8 15 0.1 0.9 0.0
212 15 22 961800 1779 767 89 12.1 13.4 4.5 14 0.9 0.5 0.0
213 16 22 908059 1754 806 85 12.3 13.1 5.5 13 0.0 -0.2 0.0
214 17 11 655907 1430 714 78 12.6 12.3 3.9 12 0.5 -0.2 0.0
215 18 0 0 0 0 0 0.0 0.0 0.0 0 0.0 0.0 0.0
216 ================================================================================
217 All 627 828911 1465 778 84 13.8 11.0 3.4 13 0.0 0.1 0.0
```

```
218 ================================================================================
219 Normal: 648, Special: 90, Reclassified as partial: 1
220 Integrate: ...done.
221
```

Appendix C: Sample Log Files

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```
222
223 *** dtintegrate ***
224 ============================================================
225 Summary of results for scan rotation from 24.000 to 29.000
226 with image sequence numbers from 1 to 20
227 ------------------------------------------------------------
228
229 Total reflections predicted: 2714
230 Total reflections with no errors: 1687
231 Total reflections with bad errors*: 64
232 Total reflections partial in scan*: 886
233 Total reflections unprocessed at end: 0
234 Total reflection profiles written: 1764
235
236 Reflection integration status codes
237 ====================================
238 Status Num reflns
239 ------------------------------------
240 No Errors: 1687
241 ------------------------------------
242 Processed special: 158 Not processed as strong, but otherwise OK
243 On edge 0: 2 Some intensity on edge of box in 1st dim
244 On edge 1: 0 Some intensity on edge of box in 2nd dim
245 On edge 2: 78 Some intensity on edge of box in 3rd dim
246 Too far 0: 0 Obs centroid too far from calc in 1st dim
247 Too far 1: 0 Obs centroid too far from calc in 2nd dim
248 Too far 2: 0 Obs centroid too far from calc in 3rd dim
249 Too big 0: 0 Obs size too large in 1st dim
250 Too big 1: 0 Obs size too large in 2nd dim
251 Too big 2: 0 Obs size too large in 3rd dim
252 Overlap 0: 0 *Obs peak overlapped in 1st dim
253 Overlap 1: 0 *Obs peak overlapped in 2nd dim
254 Overlap 2: 0 *Obs peak overlapped in 3rd dim
255 Too dark: 64 *Some peak pixels saturated
256 Too low: 0 *Some peak pixels too low, may be shadowed
257 Bad background: 0 *Error in background determination
258 Bad background sd: 0 *Error in background sigma determination
259 Bad non-uniformity A: 0 *Peak pixels flagged as bad
260 Bad non-uniformity B: 0 Background pixels flagged as bad
261 Partial at scan start: 513 *Reflns incomplete at start of the rotation
262 Partial at scan end: 393 *Reflns incomplete at end of the rotation
263 Rotation too wide: 0 *Reflns predicted to be on too many images
264 ====================================
265 *Rejected from output.
266
267 dtintegrate: There were 1764 profiles written to file reflnprofiles.profit.
268
269 dtprofit: Copyright (c) 1996 Molecular Structure Corporation
270 dtprofit settings:
271
272 Minimum required contributors to a reference profile: 50
273 Minimum reference profile value in peak area: 0
274 Variance weighted profile analysis method B used.
275 Maximum number of reference profiles: 72
276 Number of reflection profiles read in: 1764
277 Profile Reflns Sum(Pi**2/Vi) Contributors
278 ============================================
```

```
279 0 149 670 0 0/0 18/0 1/1 6/0 19/6 24/0 7/21 25/121
280 1 149 670 1 1/1 19/6 7/21 2/0 6/0 0/0 25/121
281 ...
282 71 193 648 71 71/0 53/0 70/12 65/0 52/8 47/0 64/173
283 72 1764 620 Overall profile
284 File D0001.refprof successfully opened.
285 Success writing file D0001.refprof!
286 File D0019.refprof successfully opened.
```

Appendix C: Sample Log Files


```
287 Success writing file D0019.refprof!
288 File D0037.refprof successfully opened.
289 Success writing file D0037.refprof!
290 File D0055.refprof successfully opened.
291 Success writing file D0055.refprof!
292
293 Int/SigmaI vs Average correlation of
294 observed to reference profiles
295 ====================================
296 Sigma range Avg.Corr. Num.Refln.
297 ------------------------------------
298 0 ... 3 0.169 31
299 3 ... 6 0.636 52
300 6 ... 9 0.845 65
301 9 ... 12 0.926 142
302 12 ... 15 0.954 286
303 15 ... 18 0.970 279
304 18 ... 21 0.978 245
305 21 ... 24 0.983 219
306 24 ... 27 0.988 149
307 27 ... 30 0.993 296
308 ------------------------------------
309
310 Correlation range vs
311 number of reflections
312 ========================
313 Corr.range Num.Refln.
314 ------------------------
315 0.0 ... 0.1 7
316 0.1 ... 0.2 8
317 0.2 ... 0.3 6
318 0.3 ... 0.4 7
319 0.4 ... 0.5 9
320 0.5 ... 0.6 14
321 0.6 ... 0.7 13
322 0.7 ... 0.8 25
323 0.8 ... 0.9 71
324 0.9 ... 1.0 1604
325 ------------------------
326 Number of reflections written: 1764
327 DTREK_STATUS: 0
```

Lines 14-25 The command line options/settings are listed.

Line 27 The 3D method is used, rather than the 2D method. (The 2D method is not available at this time.)

Line 28 The non-uniformity type (see section 4.5 and p. 17) is None.

Line 30 The first image is read in.

Lines 34-37 The name of the image, current date, and time are listed.

Lines 40-44 The rotation start, end, increment, and exposure time are listed.

Lines 46-50 The numbers of new, active, full, done normal and done special reflections are listed. New reflections are those for which the 3D integration box is newly created.

Active reflections includes all reflections which receive any pixel contributions from the current image. Full reflections are those for which the 3D integration box has just filled. DNormal reflections are those full reflections (from this image or a previous image, but within a batch) which have a normal preliminary integration. DSpecial reflections are those full reflections which have a special preliminary integration and which do not have an accurate centroid determination. A special integration might occur if the reflection is not strong or a warning or error occurred during integration.

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Lines 52-56 The total number of allocated 3D shoeboxes (a shoebox is the 3D data array of pixels for a single reflection) is listed, the number that are filling (i.e. in use), those that are full, and those that are freed (not in use), are listed. Full shoeboxes are buffered until the end of a batch when refinement is done and profiles are written out.

Line 58 A big portion of the output log file was edited away.

Lines 59-85 The last image in the scan to integrate is read in and info about it is listed.

Lines 86-87 The end-of-batch refinement is about to take place. The refinement options are listed.

Lines 88-191 The standard refinement output is listed. For an explanation, see section 4.8.

Lines 184-185 Notice that the residuals are very low since 3D centroids are used in refinement.

Lines 194-218 Information about strong peaks is listed for 18 different areas of the detector. The detector is divided into 6 by 3 areas (fast pixel direction by slow pixel direction). The columns are:

Num Number of strong reflections

Intensity Average intensity of strong reflections

Sigma Average standard deviation of intensity

BackAvg Average background value

BackSig Average background standard deviation

Siz0 Average peak size at 1σ in pixels in the fast pixel direction

Siz1 Average peak size at 1σ level in pixels in the slow pixel direction

Siz2 Average peak size at 1σ level in images in rotation direction

Dl Average spot size as a function in reciprocal space

Shft0 Average shift in pixels between observed and calculated centroid in the fast pixel direction

Shft1 Average shift in pixels between observed and calculated centroid in the slow pixel direction

Shft2 Average shift in images between observed and calculated centroid in the rotation direction

The calculated centroid of non-strong reflections is shifted by the above shifts.

Line 219 The number of reflections processed in the batch is listed.

Line 220 The end of images is reached and integration is done.

Lines 225-265 A summary of the number of reflections integrated, along with their status, is listed. Reflections with bad errors and that are partial are not included in the output reflection files. The status codes are self-explanatory. A reflection that is partial at both the scan start and scan end is counted in both places, but counted only once at

the top. Reflections in categories that are asterisked (*) are rejected. Reflections may fit in multiple categories.
Line 267 The number of reflection profiles written to reflnprofiles.profit is listed. These profiles will be read by dtprofit and processed.

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Lines 269-270 The dtprofit module is started in order to fit profiles. This performs threedimensional profile analysis with a method similar to that of Kabsch (1988).
Line 272 At least 50 strong reflections must contribute to a reference profile. If too few reflections are found in the same region, nearby regions are used until sufficient strong reflections contribute.
Line 274 A variance weighted profile analysis method is used. This is different from Kabsch (1988), but like Otwinowski & Minor (1997).
Line 275 In this scan, there are up to 72 regions (18 per detector * 4 batches) for which reference profiles are calculated.
Lines 277-282 For each regional reference profile the number of strong reflections that contribute and their original region (as m/n pairs) are listed. If too few strong reflections are found, all strong reflections in the input are used.
Line 283 A single overall reference profile is also calculated.
Lines 284-291 The reference profiles are written to disk in the form of a d*TREK image file. Each image file shows 18 reference profiles. Each reference profile is a three-dimensional cube of 9 by
9 by 9 Kabsch-transformed pixels. The pixels are NOT in image or data space, but rather in a transformed Kabsch space (read his 1988 paper *J. Appl. Cryst.* **21**, 916-924). Since images are displayed
in 2D, each 9 by 9 by 9 cube is displayed as a series of 9 two-dimensional 9 by 9 planes (Figures 19-22).

Reference profiles.
Profile size too large. Peak crowded into center, so decrease first Profile size value (make box smaller).
Profile size too small. Peak overfills box, so increase first Profile size value (make box bigger).
Profile size just right. Peak fills box, but there is background at edges and faces.

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Stack them up in your mind to make them 3D. Because of the Kabsch transformation, reference profiles
should look very similar throughout reciprocal space. The appearance of the reference profiles is affected by the **Profile size** option. The width of the profile in the plane of the display is determined by
the first value to **Profile size** , while the number of squares the profile fits in is determined by the second
value. To make the profiles appear larger in the plane, decrease the first value. To make them appear

smaller, increase the first value. To make them appear on more squares, decrease the second value. To
make them appear on fewer squares, increase the second value. In reality, the profiles do not change physical size — you change the size of the box around them. That is, by cropping the box closer to the
profile, the profile will fill a larger portion of the box. If you make the box larger, the profile will fill a
smaller portion of the box. In any event, do not make the second value less than 2 times the image rotation angle increment!
Lines 293-308 The average correlation between observed profiles and the corresponding reference profile is listed for 10 Intensity/SigmaI ranges. If the assumptions of profile -fitting
are valid, then the correlations should be very high (>0.85) for strong reflections.
You are reminded that the assumptions are: 1) Reflection centroids are accurately
predicted; and 2) Reflections ***do*** have the same profiles, that is, the same shape and
boundary *and* the same relative intensity distribution within the boundary.

Laue Log

```
1 dtcell: Molecular Structure Corporation
2 d*TREK version 6.2SSI -- Dec 11 2000
3 Command line:
4 dtcell input.head dtintegrate.ref -head output.head -tols 1e6 1e6 1e6 \
5 1e6 1e6 1e6 -anom -maxrmerge 0.150000 -spacegroup 16 -laueonly
6 Header "input.head" opened.
7 Header of file input.head successfully read.
8 Lattice oP assumed for space group 16.
9 Command line string: >>-head<<
10 Output Header Name set to "output.head".
11 Command line string: >>-tols<<
12 Cell tolerances set to [ 1000000.00 1000000.00 1000000.00 1000000.00
13 1000000.00 1000000.00]
14 Command line string: >>-anom<<
15 Laue check assumes I+ != I-
16 Command line string: >>-maxrmerge<<
17 Maximum R-merge is 0.150000
18 Command line string: >>-spacegroup<<
19 Space group set to: P222 (#16)
20 Laue check disabled.
21 Laue group set to: mmm
22 Lattice set to oP
23 Command line string: >>-laueonly<<
//////////////////////////////
24 Finished reading command line.
25 Input Cell: [ 6.36 15.51 25.07 90.00 90.00 90.00 ]
26 Input Sigmas: [ 0.0003 0.0009 0.0013 0.0000 0.0000 0.0000 ]
27 Input Orientation: [ 97.41 -1.70 171.25 ]
28 Reading Reflection file dtintegrate.ref ...
29 Creflnlist::nRead with filename: dtintegrate.ref
30 INFO in Creflnlist::nRead, EOF after 12641 reflections read in
31 (12641 total now in list).
32 Laue Check
-----------------------------------------------------
33 Laue Unique Num Calc Obs R-Merge Pass?
34 class axis unique mult mult
-----------------------------------------------------
35 -1 - 1314 1 2.01 0.02 [PASS]
36 2/m a 3786 2 2.25 0.02 [PASS]
37 2/m b 4037 2 2.29 0.02 [PASS]
38 2/m c 1996 2 2.13 0.02 [PASS]
```

```
39 mmm - 4195 4 2.45 0.02 [PASS]
40 4/m a 3091 4 2.53 0.43 ------
41 4/m b 2186 4 2.45 0.33 ------
42 4/m c 3504 4 2.87 0.32 ------
43 4/mmm a 3213 8 3.40 0.44 ------
44 4/mmm b 2532 8 2.81 0.30 ------
45 4/mmm c 2732 8 4.10 0.33 ------
46 -3 - 2782 3 2.58 0.59 ------
47 -3m1 - 2979 6 3.23 0.65 ------
48 -31m - 3169 6 3.25 0.64 ------
49 6/m - 2947 6 3.44 0.53 ------
50 6/mmm - 2310 12 4.75 0.64 ------
51 m-3 - 3276 12 3.17 0.54 ------
52 m-3m - 2557 24 4.39 0.69 ------
-------------------------------------------------------
53 mmm selected with R-merge of ..... 0.02
54 No reindexing done.
55 Reflection file not updated.
56 Header "output.head" written.
```

Centricity Log

```
1 dtcell: Molecular Structure Corporation
2 d*TREK version 6.2SSI -- Dec 11 2000
3 Command line:
4 dtcell input.head dtintegrate.ref -head output.head -centricityonly
5 Header "input.head" opened.
6 Header of file input.head successfully read.
7 Lattice oP assumed for space group 16.
8 Command line string: >>-head<<
9 Output Header Name set to "output.head".
10 Command line string: >>-centricityonly<<
//////////////////////////////
11 Finished reading command line.
12 Input Cell: [ 6.36 15.51 25.07 90.00 90.00 90.00 ]
13 Input Sigmas: [ 0.0003 0.0009 0.0013 0.0000 0.0000 0.0000 ]
14 Input Orientation: [ 97.41 -1.70 171.25 ]
15 Reading Reflection file dtintegrate.ref ...
16 Creflnlist::nRead with filename: dtintegrate.ref
17 INFO in Creflnlist::nRead, EOF after 12641 reflections read in
(12641 total now in list).
18 N(Z) test: fraction of intensities less than Z x <I>
-------------------------------------------------------------------------------
19 Z= 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
20 centric .248 .345 .419 .479 .520 .561 .597 .629 .657 .683
21 acentric .095 .181 .259 .330 .394 .451 .503 .551 .593 .632
22 deviation -.153 -.164 -.160 -.149 -.126 -.110 -.094 -.078 -.064 -.051
23 theoretical average deviation ==> -.115
24 measured 0.317 0.463 0.556 0.617 0.665 0.698 0.723 0.745 0.766 0.781
25 deviation -0.069 -0.118 -0.137 -0.138 -0.145 -0.137 -0.126 -0.116 -0.109 -0.098
26 measured average deviation ==> -0.119
-------------------------------------------------------------------------------
27 Centric Distribution Selected.
28 No reindexing done.
29 Reflection file not updated.
30 Header "output.head" written.
31
```

Spacegroup Log

```
1 dtcell: Molecular Structure Corporation
2 d*TREK version 6.2SSI -- Dec 11 2000
3 Command line:
4 dtcell input.head dtintegrate.ref -head output.head -lauegroup mmm \
5 -acentric -rejects 20 -asigma 10.000000
6 Header "input.head" opened.
7 Header of file input.head successfully read.
8 Lattice oP assumed for space group 16.
```

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```
9 Command line string: >>-head<<
10 Output Header Name set to "output.head".
11 Command line string: >>-lauegroup<<
12 Laue group set to: mmm
13 Laue check disabled.
14 Command line string: >>-acentric<<
15 Space group is Acentric.
16 Centricity check disabled.
17 Command line string: >>-rejects<<
18 Command line string: >>-asigma<<
19 Absence I/Sigma(I) set to 10.000000
20 ////////////////////////////
21 Finished reading command line.
22 Input Cell: [ 6.36 15.51 25.07 90.00 90.00 90.00 ]
23 Input Sigmas: [ 0.0003 0.0009 0.0013 0.0000 0.0000 0.0000 ]
24 Input Orientation: [ 97.41 -1.70 171.25 ]
25 Reading Reflection file dtintegrate.ref ...
26 Creflnlist::nRead with filename: dtintegrate.ref
27 INFO in Creflnlist::nRead, EOF after 12641 reflections read in
28 (12641 total now in list).
29 Checking systematic absences...
30 Outputing 'dtcell_rejects.ref'...
31 Number of reflections written: 3724
32 BEGIN Texsan Output
--------------------------------------------------------------------------------
33 Odd/Even parity class
--------------------------------
34 Class Total Observed <I/sig>
--------------------------------
35 eee 1606 1364 160.9
36 eeo 1593 1325 166.6
37 eoe 1576 1295 169.2
38 eoo 1571 1362 174.5
39 oee 1572 1362 164.9
40 oeo 1573 1380 155.4
41 ooe 1572 1378 181.8
42 ooo 1578 1404 183.3
--------------------------------
-------------------------------- --------------------------------
43 hk0 Total Observed <I/sig> h0l Total Observed <I/sig>
-------------------------------- --------------------------------
44 ee 83 68 367.3 e e 102 79 258.4
45 eo 74 44 222.4 e o 101 62 105.3
46 oe 78 63 296.6 o e 103 85 276.9
47 oo 77 53 250.1 o o 100 80 208.8
-------------------------------- --------------------------------
-------------------------------- --------------------------------
48 0kl Total Observed <I/sig> hhl Total Observed <I/sig>
-------------------------------- --------------------------------
49 ee 374 287 185.4 e e 97 89 380.6
50 eo 372 291 181.9 e o 98 73 357.0
51 oe 354 266 217.1 o e 96 90 378.7
52 oo 360 284 257.4 o o 94 88 434.2
-------------------------------- --------------------------------
--------------------------------
53 h-hl Total Observed <I/sig>
--------------------------------
54 ee 114 98 236.7
55 eo 113 77 183.4
56 oe 113 107 249.9
57 oo 117 108 304.1
--------------------------------
-------------------------------- --------------------------------
58 hhh Total Observed <I/sig> hh0 Total Observed <I/sig>
```

```
------------------------------ ------------------------------
59 e 5 5 708.6 e 5 3 496.1
60 o 7 7 1008.4 o 5 5 919.9
```



```
------------------------------ ------------------------------
------------------------------ ------------------------------
61 h00 Total Observed <I/sig> 0k0 Total Observed <I/sig>
------------------------------ ------------------------------
62 e 4 4 914.1 e 19 19 744.1
63 o 4 4 75.9 o 18 1 -0.5*
64 o/e -- -- 0.1 o/e -- -- -0.0
------------------------------ ------------------------------
--------------------------------
65 00l Total Observed <I/sig>
--------------------------------
66 e 18 15 383.6
67 o 19 2 3.0*
68 o/e -- -- 0.0
--------------------------------
-------------------------------------------------------------
69 Zone a+b=4n a+b not equal 4n
70 Total Observed <I/sig> Total Observed <I/sig>
-------------------------------------------------------------
71 0kl 366 287 214.7 1094 841 208.4
72 h0l 101 79 230.6 305 227 206.9
73 hk0 79 60 269.9 233 168 291.9
-------------------------------------------------------------
74 Zone a=4n a not equal 4n
75 Total Observed <I/sig> Total Observed <I/sig>
-------------------------------------------------------------
76 0k0 10 10 572.2 27 10 311.3
77 00l 9 7 351.1 28 10 135.8
78 h00 1 1 75.4 7 7 555.0
-------------------------------------------------------------
-------------------------------------------------------------
79 Zone 2h+l=4n 2h+l not equal 4n
80 Total Observed <I/sig> Total Observed <I/sig>
-------------------------------------------------------------
81 hhl 96 87 288.7 289 253 419.9
-------------------------------------------------------------
-----------------------------------------------------------------------
82 h+l=3n;l odd h+l=3n h+l not equal 3n
83 Total Obsvd <I/sig> Total Obsvd <I/sig> Total Obsvd <I/sig>
-----------------------------------------------------------------------
h-h0l 76 60 240.0 154 131 239.8 303 259 246.1
-----------------------------------------------------------------------
84 -h+l=3n;l even -h+l=3n -h+l not equal 3n
-----------------------------------------------------------------------
85 h-h0l 77 60 231.2 149 125 238.2 308 265 246.8
-----------------------------------------------------------------------
-------------------------------------------------------------
86 l=3n l not equal 3n
87 Total Observed <I/sig> Total Observed <I/sig>
-------------------------------------------------------------
88 000l 13 6 212.5 24 11 175.0
-------------------------------------------------------------
89 l=6n l not equal 6n
-------------------------------------------------------------
90 000l 6 5 457.0 31 12 136.2
-------------------------------------------------------------
-------------------------------------------------------------------------
91 END Texsan Output
92 ALL Systematic Absences
-------------------------------------------------------------------------
```

```
93 Refln. Type hkl 0kl h0l hk0 h00 0k0 00l
-------------------------------------------------------------------------------
94 Total Reflns 12641 1460 406 312 8 37 37
95 h!=2n 6295 ------ 203 155 4 ------ ------
96 5524 ------ 165 116 4 ------ ------
97 171.35 ------ 243.36 273.47 75.91 ------ ------
98 h=2n 6346 ------ 203 157 4 ------ ------
99 5346 ------ 141 112 4 ------ ------
100 167.79 ------ 182.22 299.00 914.12 ------ ------
101 k!=2n 6297 714 ------ 151 ------ 18 ------
102 5439 550 ------ 97 ------ 1 ------
103 177.22 237.42 ------ 236.50 ------ -0.55* ------
104 k=2n 6344 746 ------ 161 ------ 19 ------
105 5431 578 ------ 131 ------ 19 ------
106 161.95 183.65 ------ 333.05 ------ 744.09 ------
107 l!=2n 6315 732 201 ------ ------ ------ 19
108 5471 575 142 ------ ------ ------ 2
109 169.97 219.01 156.79 ------ ------ ------ 3.01*
110 l=2n 6326 728 205 ------ ------ ------ 18
11 5399 553 164 ------ ------ ------ 15
169.15 200.83 267.70 ------ ------ ------ 383.64
112 k+l!=2n 6314 726 ------ ------ ------ ------ ------
113 5378 557 ------ ------ ------ ------ ------
114 168.25 199.05 ------ ------ ------ ------ ------
115 k+l=2n 6327 734 ------ ------ ------ ------ ------
116 5492 571 ------ ------ ------ ------ ------
117 170.87 220.72 ------ ------ ------ ------ ------
118 h+l!=2n 6308 ------ 204 ------ ------ ------ ------
119 5427 ------ 147 ------ ------ ------ ------
120 171.94 ------ 191.95 ------ ------ ------ ------
121 h+l=2n 6333 ------ 202 ------ ------ ------ ------
122 5443 ------ 159 ------ ------ ------ ------
123 167.19 ------ 233.84 ------ ------ ------ ------
124 h+k!=2n 6292 ------ ------ 152 ------ ------ ------
125 5399 ------ ------ 107 ------ ------ ------
126 166.00 ------ ------ 260.44 ------ ------ ------
127 h+k=2n 6349 ------ ------ 160 ------ ------ ------
128 5471 ------ ------ 121 ------ ------ ------
129 173.09 ------ ------ 310.90 ------ ------ ------
130 h!=4n 9572 ------ 310 229 7 ------ ------
131 8376 ------ 244 172 7 ------ ------
132 175.36 ------ 239.44 293.55 554.96 ------ ------
133 h=4n 3069 ------ 96 83 1 ------ ------
134 2494 ------ 62 56 1 ------ ------
135 151.46 ------ 126.74 266.36 75.42 ------ ------
136 k!=4n 9469 1097 ------ 231 ------ 27 ------
137 8188 842 ------ 167 ------ 10 ------
138 176.10 220.86 ------ 285.36 ------ 311.34 ------
139 k=4n 3172 363 ------ 81 ------ 10 ------
140 2682 286 ------ 61 ------ 10 ------
150.05 176.98 ------ 289.04 ------ 572.17 ------
141 l!=4n 9468 1096 302 ------ ------ ------ 28
142 8175 857 223 ------ ------ ------ 10
143 168.43 213.57 210.68 ------ ------ ------ 135.82
144 l=4n 3173 364 104 ------ ------ ------ 9
```

Appendix C: Sample Log Files


```
145 2695 271 83 ------ ------ ------ 7
146 172.94 199.04 218.93 ------ ------ ------ 351.10
147 k+l!=4n 9481 1094 ------ ------ ------ ------ ------
148 8124 841 ------ ------ ------ ------ ------
149 170.07 208.38 ------ ------ ------ ------ ------
150 k+l=4n 3160 366 ------ ------ ------ ------ ------
151 2746 287 ------ ------ ------ ------ ------
152 168.02 214.65 ------ ------ ------ ------ ------
```

```
153 h+l!=4n 9474 ------ 305 ------ ------ ------ ------
154 8151 ------ 227 ------ ------ ------ ------
155 170.61 ------ 206.89 ------ ------ ------ ------
156 h+l=4n 3167 ------ 101 ------ ------ ------ ------
157 2719 ------ 79 ------ ------ ------ ------
158 166.43 ------ 230.61 ------ ------ ------ ------
159 h+k!=4n 9476 ------ ------ 233 ------ ------ ------
160 8137 ------ ------ 168 ------ ------ ------
161 166.99 ------ ------ 291.90 ------ ------ ------
162 h+k=4n 3165 ------ ------ 79 ------ ------ ------
163 2733 ------ ------ 60 ------ ------ ------
164 177.26 ------ ------ 269.86 ------ ------ ------
-------------------------------------------------------------------------------
165 Sending tcl command
166 Systematic Absences <I/sig(I)> <= 10.00
-------------------------------------------------------------------------------
167 Refln. Type hkl 0kl h0l hk0 h00 0k0 00l
-------------------------------------------------------------------------------
168 Total Reflns 12641 1460 406 312 8 37 37
169 Condition ---- ---- ---- ---- ---- k!=2n l!=2n
170 Num Reflns. ---- ---- ---- ---- ---- 18 19
171 Num Observed ---- ---- ---- ---- ---- 1 2
172 <I/sig(I)> ---- ---- ---- ---- ---- -0.55 3.01
-------------------------------------------------------------------------------
173 Sending tcl command
174 Spacegroups found.
--------------------------------------------------
175 Number Name Presentation Centricity Likelihood
--------------------------------------------------
176 18 P21212 P22121 Acentric 1.00
--------------------------------------------------
177 Space groups whose 'Presentation' field differs
178 from the 'Name' field were found in a
179 non-standard presentation.
180 Re-indexing will be required to convert to a
181 standard presentation.
182 Options:
183 T) Print Texsan Output
184 S) Print Selected Spacegroups
185 A) Print Table of absences used to selected spacegroups
186 B) Print Table of all absences applicable to laue group
187 Q) Quit
188 #) Type spacegroup number.
189 Enter) Select spacegroup 18
190 Choice: Q
191 Terminating.
192 No reindexing done.
193 Reflection file not updated.
194 Header "output.head" written.
```

Scale and Average Log

Appendix C: Sample Log Files

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```
1 dtscalemerge: Copyright (c) 1996 Molecular Structure Corporation
2 Header of file lyso.head successfully read.
3 Creflnlist::nRead called.
4 Names of reflection fields:
5 nH (int)
6 nK (int)
7 nL (int)
8 nPartial (int)
9 nBatchIndex (int)
10 nPackedHKL (int)
11 nReducedH (int)
12 nReducedK (int)
13 nReducedL (int)
```

```
14 nAnomFlag (int)
15 nCentPhase (int)
16 fIntensity (float)
17 fSigmaI (float)
18 fObs_pixel0 (float)
19 fObs_pixel1 (float)
20 fObs_rot_mid (float)
21 f2STLsq (float)
22 fResolution (float)
23 sBatch (Cstring)
24 INFO in Creflnlist::nRead, EOF after 31914 reflections read in (31914 total now
25 in list).
```

Lines 1-25 The input reflection list is read in and the fieldnames in the reflection list are listed. Note that for efficiency, the fields normally added by dtscalemerge are present in the reflection list. If not present, they would be added, but this would take additional time.

```
27 Cscalemerge listing:
28 Batch fixed: L002
29 Scale fixed: 1
30 Bvalue fixed: 0
31 Rej criteria: 3
32 Mul sig fact: 1.3
33 Add sig fact: 0.02
34 Max cycles: 10
35 FixB Flag: 0
36 Anom Flag: 0
```

Lines 27-36 The option settings used by this run of dtscalemerge are listed. These confirm what is set on the command line or in the **Scale** menu.

```
37 Crystal listing:
38 Unit cell lengths: 79.2, 79.2, 38.9
39 Unit cell angles: 90, 90, 90
40 Unit cell volume: 244006
41 Spacegroup number: 96
42 name: P43212
43 Num. equiv. posns: 8
```

Lines 37-43 Information about the crystal unit cell dimensions and spacegroup is listed next. This comes from the `input_header_file` which in this example is `lyso.head`.

```
44 There are 20 different batches in the input reflection list.
```


Line 44 20 different batch names were found in the input reflection list.

```
45 Observed position limits of the Batches
46 ------------------------------------------------------------------------------
47 Batch Num fObs_pixel0 fObs_pixel1 fObs_rot_mid
48 name refs Min Max Min Max Min Max
49 ------------------------------------------------------------------------------
50 L001 1603 -96.0 95.2 -91.6 85.8 -28.8 -28.8
51 L002 1625 -95.2 95.0 -88.9 90.0 -26.3 -26.3
...
68 L019 1564 -96.0 94.9 -94.8 93.9 16.3 16.3
69 L020 1590 -95.7 94.8 -91.4 93.1 18.8 18.8
70 ------------------------------------------------------------------------------
```

Lines 45-70 A table lists for each batch the minimum and maximum value of the observed reflection positions found in the input reflection list file. In this example, the `fObs_pixel0` and `fObs_pixel1` fields are in millimeters and not pixels. This table is a quick check that the input reflection list contains the expected range of values.

```
71 Intensity and Resolution limits of the Batches
72 ------------------------------------------------------------------------------
73 Batch Num Intensity Resolution [2sinT/lam]^2
74 name refs Min Max Min Max Min Max
75 ------------------------------------------------------------------------------
76 L001 1603 -26.7 11964.6 39.60 1.94 0.0006 0.2646
```

```
77 L002 1625 -16.5 13621.4 79.20 1.95 0.0002 0.2642
...
94 L019 1564 -26.6 14997.3 27.75 1.94 0.0013 0.2653
95 L020 1590 -33.7 12513.4 27.75 1.94 0.0013 0.2647
96 ------------------------------------------------------------------------------
```

Lines 71-96 The minimum and maximum intensity, resolution and $|d^*|^2 \equiv (2\sin\theta/\lambda)^2$ for each batch is listed in this table. Check that the minimum intensity of each batch is not outrageously less than zero; this would indicate problems with integration. Confirm that the resolution limits are what is expected.

```
97 Sorting and reducing reflnlist to asymmetric unit ...
98 ... done sorting
```

Lines 97-98 The reflection list was reduced to the asymmetric unit and sorted. The input list need not be sorted as this step will ensure that symmetry-related reflections are adjacent in the file.

```
99 Selection string: -fIntensity/fSigmaI<3.000
100 Number of reflns which match above selection: 5294
```

Lines 99-100 This confirms that you excluded refle ctions with $I/\sigma < 3$ from contributing to the refinement of the scale factors. 5294 of the input reflections were thus excluded. These reflections are included, however, in the final statistics.

```
101 Last cycle: no shifts.
102 For cycle number 10
```

Appendix C: Sample Log Files

Lines 101-102 The last cycle was reached, so no shifts were applied. Dtscalemerge calculates and prints out statistics on the results.

```
103 Method 1 Expected Rmerge: 0.033
104 Method 2 Expected Rmerge: 0.034
105 Actual Rmerge: 0.032
```

Lines 103-105 Two methods for approximating the *Rmerge* are given, followed by the actual *Rmerge* (see the equation below) in the data set. The actual *Rmerge* should be close to the expected *Rmerge*s or something is wrong with the error model. The expected *Rmerge*s are calculated as follows:

Method 1: $Rmerge\ I_h = 1$, where I_h is the average intensity for all averaged reflections.

Method 2: $Rmerge = \frac{\sum_h \sum_i \sigma_h}{\sum_h \sum_i I_h}$, where σ_h is the average standard deviation for averaged reflections, N_h is the number of unique reflections, and N_i is the number of overlaps.

Actual: $Rmerge = \frac{\sum_h \sum_i |I_{hi} - I_h|}{\sum_h \sum_i I_h}$

$\sum\sum$ –
$\sum\sum$
| |
```
106 Multiplicity of observed reflections
107 ------------------------------------------------------------------------------
108 Mult | 1 2 3 4 5 6 7 8 >8
109 ------------------------------------------------------------------------------
110 Refs | 897 2720 3418 2628 2060 1492 500 142 20
111 ------------------------------------------------------------------------------
112 *Reflections with a multiplicity of 1 are not used in
113 scale factor refinement nor in Rmerge calculations.
```
Lines 106-113 The multiplicity of observed reflections is listed in a table. The entire process of refining scale factors requires multiple observations for reflections. That is, reflections that are symmetry-related need to appear in multiple batches. Reflections with a multiplicity of 1 are neither used in scale factor refinement nor in the *Rmerge* calculations. A high redundancy will improve the *I/*s in the merged and averaged results (see e.g. the dtscalemerge documentation Eqn. 10).
```
114 Overlaps among scaling batches
115 ------------------------------------------------------------------------
116 Batch | L001 L002 L003 L004 L005 L006 L007 L008 L009 L010
117 ------------------------------------------------------------------------
118 L001 | 298 745 671 259 196 168 199 174 182 263 | L001
119 L002 | 787 659 286 243 193 162 204 166 161 280 | L002
120 L003 | 656 226 240 246 217 173 162 162 191 259 | L003
```
...
```
163 L020 | 137 172 151 166 178 166 198 169 191 134 | L020
```

```
164 ------------------------------------------------------------------------
165 Batch | L011 L012 L013 L014 L015 L016 L017 L018 L019 L020
166 ------------------------------------------------------------------------
```
Lines 114-166 Overlaps among the scaling batches are listed next (but only if the dtscalemerge command line option `-countoverlap` was used). The entire refinement of scale factors depends on overlaps among the different batches. If a batch has no overlaps with the other batches, then there is no information present in the reflection list which can be used to refine the scale factor of that batch. In this case, the procedure used in the nonlinear least squares algorithm will simply keep the scale factor for that batch unchanged.
Note that this table is normally **NOT** symmetric. For example, there are 745 reflections in batch `L001` that have at least 1 symmetry-related reflection in batch `L002`. But there are 787 reflections in batch `L002` that have symmetry mates in `L001`. There are 298 reflections in `L001` which overlap with a symmetry-related reflection in the same batch (each reflection is counted once). To make this excrutiatingly clear, here is another example: suppose batch `X001` has 10 copies of a reflection with *hkl* = (10 1 2) and batch `X002` has just 1 copy. The table will then appear:
```
--------------------
Batch | X001 X002
--------------------
X001 | 10 10
X002 | 1 0
```
If a batch has few overlaps, you might use dtreflnmerge or an editor to combine that batch with another batch that you think will have the same scale factors (i.e. a batch that is adjacent in rotation angle or time scan; see section 4.13).
```
167 Reflections in input file
168 ------------------------------------------------------------------------------
```

```
169 Batch Num Num Num Num Num
170 name refs excluded rejs ovlps singles
171 ------------------------------------------------------------------------------
172 L001 1603 206 53 1327 17
173 L002 1625 227 40 1341 17
174 L003 1609 238 34 1310 27
175 L004 1574 238 25 1280 31
...
191 L020 1590 268 28 1152 142
192 ------------------------------------------------------------------------------
193 All batches 31914 5294 585 25138 897
```

Lines 167-193 Information about reflections in the batches is listed in a table.

`Num refs` Total number of reflections in this batch

`Num excluded` Number of reflections excluded because of the *I/*σ cutoff.

`Num rejs` Number of rejected reflections. There should be very few, if any rejected reflections. Any batch with a large number of rejected reflections should be investigated. Perhaps it is indexed differently from the other batches.

`Num ovlps` Number of reflections in this batch which overlap another reflection either in this batch or another batch.

`Num singles` Number of reflections with no overlaps in the entire dataset. To have many of these is undesirable . One observation for a data point, as opposed to numerous, is not recommended.

```
194 Refined scale factors
```

Appendix C: Sample Log Files


```
195 ------------------------------------------------------------------------------
196 Batch Num Scale
197 name ovlps K *Shifts B *Shifts
198 ------------------------------------------------------------------------------
199 L001 1327 1.0138 0.0000 0.0389 0.0000
200 L002 1341 1.0000 0.0000 0.0000 0.0000
201 L003 1310 0.9911 0.0000 -0.0036 0.0000
...
216 L018 1203 1.0519 0.0000 -0.3011 0.0000
217 L019 1149 1.0593 0.0000 -0.3365 0.0000
218 L020 1152 1.0748 0.0000 -0.3388 0.0000
219 ------------------------------------------------------------------------------
220 *Shifts are for previous cycle only!
```

Lines 194-220 This table lists the refined scale factors for the batches and the number of reflections that contributed to the refinement. Examine this to assure that the scale factors "make sense." In this example, an unfrozen lysozyme crystal was used. Some radiation damage is expected, but not much. That is, the later batches will need to be "scaled up" and to have larger scale factors. Indeed, this is the case. Remember that:

$$I_{hkl} = I_{corr\,hkl} \times B_j e^{-2\sin^2\theta/\lambda^2}$$

Also, since the batches are from the same crystal and same experiment, expect the scale factors to vary relatively smoothly. Indeed, this is the case. However, if the crystal had been a plate, or larger than the beam, expect larger variations due to more drastic volume changes. Finally, double check that refinement has converged. The shifts should be 0 on the last cycle.

```
221 In the tables below Rmerge is defined as:
222 Rmerge = Sum Sum |Ihi - <Ih>| / Sum Sum <Ih>
223 h i h i
```

```
224 where Ihi is the ith used observation for unique hkl h,
225 and <Ih> is the mean intensity for unique hkl h.
```

Lines 221-225 A reminder of the equation for *Rmerge*.

```
226 Rmerge vs Batch
227 ------------------------------------------------------------------------------
228 Batch Average Num Num Num Num <I/ ChiSq Rmerge Rmerge
229 name counts obs rejs ovlps single sig> batch cumul
230 ------------------------------------------------------------------------------
231 L001 865 1397 53 1327 17 12.4 0.387 0.036 0.036
232 L002 997 1398 40 1341 17 15.0 0.425 0.033 0.035
233 L003 865 1371 34 1310 27 11.7 0.314 0.035 0.035
234 L004 950 1336 25 1280 31 11.8 0.282 0.029 0.033
235 L005 887 1349 31 1286 32 11.7 0.292 0.032 0.033
236 L006 1024 1368 27 1310 31 12.7 0.309 0.032 0.033
237 L007 955 1382 27 1331 24 14.5 0.352 0.035 0.033
238 L008 921 1264 20 1216 28 13.3 0.293 0.031 0.033
239 L009 955 1310 25 1257 28 11.6 0.258 0.032 0.033
240 L010 989 1373 23 1319 31 12.4 0.256 0.027 0.032
241 L011 877 1229 26 1186 17 11.3 0.275 0.034 0.032
242 L012 951 1389 24 1338 27 11.9 0.258 0.030 0.032
243 L013 931 1245 21 1189 35 11.4 0.254 0.028 0.032
244 L014 933 1384 23 1308 53 11.9 0.245 0.030 0.032
245 L015 1069 1281 24 1210 47 11.3 0.279 0.032 0.032
246 L016 968 1248 31 1162 55 11.6 0.255 0.033 0.032
247 L017 912 1362 36 1264 62 11.1 0.246 0.032 0.032
248 L018 929 1314 36 1203 75 11.3 0.260 0.032 0.032
249 L019 977 1298 31 1149 118 11.0 0.283 0.032 0.032
250 L020 859 1322 28 1152 142 11.2 0.271 0.033 0.032
```

Appendix C: Sample Log Files


```
251 ------------------------------------------------------------------------------
252 All batches 941 26620 585 25138 897 12.0 0.29 0.032 0.032
```

Lines 226-252

This table lists *Rmerge vs Batch*. It is easy to recognize any batch not matching well with the other batches.

Average counts The average counts of reflections in the batch. This includes reflections that overlap and those that do not. If you assume Poissonian counting statistics, then the expected *Rmerge* for this batch would be $1/\sqrt{I}$. So for batch L001, $1/\sqrt{865} = 0.034$ is consistent with 0.036 found.

Num refs Total number of reflections in this batch.

Num rejs Number of rejected reflections. There should be very few, if any rejected reflections. Any batch with a large number of rejected reflections should be investigated. Perhaps the batch is indexed differently from the other batches.

Num ovlps Number of overlapping reflections in this batch that have symmetry-related mates and that contributed to the *Rmerge*.

Num singles Number of reflections with no overlaps in the entire dataset. One observation for a data point, as opposed to numerous, is not recommended.

<I/sig> The average Intensity/SigmaI for reflections in the batch. This is for the corrected but unmerged reflections. A higher `<I/sig>` was expected for the averaged reflections shown in subsequent tables.

ChiSq This is the pseudo-normalized χ^2 for each batch.

$$c\,2\,1\left(\ \right)^2$$

$$= \sum\sum - N$$
$$w\ I\ I$$
$$hi$$
$$hi\ hi\ h$$
$$i$$
$$N$$
$$h$$
$$N_{h\ hi}$$

Rmerge batch This is the *Rmerge* of the reflections which belong to this batch where I_h is calculated from reflections from all batches.

Rmerge cumul This is the *Rmerge* of the reflections which belong to this batch and all previous batches in the table where I_h is calculated from reflections from all batches.

```
253 Rmerge vs Intensity/SigmaI
254 ------------------------------------------------------------------------------
255 Int/sigmaI Average Num Num Num Num <I/ ChiSq Rmerge Rmerge
256 range counts obs rejs ovlps mults sig> norm shell cumul
257 ------------------------------------------------------------------------------
258 18 - >20 1470 15510 326 15086 3407 30.9 1.225 0.029 0.029
259 16 - 18 271 1567 49 1497 384 16.0 1.133 0.057 0.029
260 14 - 16 206 1658 39 1584 421 14.0 1.032 0.065 0.030
261 12 - 14 160 1713 49 1614 447 12.0 0.939 0.073 0.030
262 10 - 12 120 1936 46 1857 536 10.0 0.852 0.088 0.031
263 8 - 10 94 1648 26 1583 512 8.0 0.601 0.092 0.031
264 6 - 8 70 1501 39 1370 520 6.0 0.416 0.114 0.032
265 4 - 6 49 813 11 547 263 3.9 0.188 0.117 0.032
266 2 - 4 --- 274 0 0 0 --- --- --- 0.032
267 < 0 - 2 --- 0 0 0 0 --- --- --- 0.032
268 ------------------------------------------------------------------------------
269 < 0 - >20 941 26620 585 25138 6490 19.5 1.00 0.032 0.032
```

Lines 253-269 This table lists *Rmerge vs Intensity/SigmaI*.

Appendix C: Sample Log Files

Average counts The average counts of reflections in the shell. This includes reflections that overlap and those that do not. If you assume Poissonian counting statistics, then the expected *Rmerge* for this shell would be $1\ I$. So, for the shell of highest *I/s*, $1\ 1470 = 0.026$ is consistent with 0.029 found. In the 4-6 shell, $1\ 49 = 0.142$ is consistent with 0.117 found.

Num obs Number of reflections in this shell.

Num rejs Number of rejected reflections. There should be very few, if any rejected reflections. Any shell with a large number of rejected reflections should be investigated. Perhaps there are a number of saturated reflections or unaccounted shadows on the detector.

Num ovlps Number of reflections in this shell having symmetry-related mates and that contributed to the *Rmerge*.

Num mults Number of unique reflections measured multiple times in the shell. The average multiplicity or redundancy for the shell is Num ovlps / Num mults.

<I/sig> The average Intensity/SigmaI for averaged reflections in the shell. As expected, there is a larger <I/sig> for the averaged reflections than shown for unaveraged reflections in the *Rmerge vs. Batch* table.

ChiSq norm This is the normalized χ_2 popularized by Dr. Zbyszek Otwinowski

calculated as

$$\chi^2 = \frac{1}{N-1}\sum_h \sum_i w_{hi}\left(I_{hi} - I_h\right)^2$$

where N_h is the number of unique reflections and N_{hi} is the number of contributors to or multiplicity of averaged reflection I_h. Values close to 1 suggest that the error model (w_{hi}) is valid.

Rmerge shell This is the *Rmerge* for reflections which belong to this shell.

Rmerge cumul This is the cumulative *Rmerge* for reflections which belong to this shell and all previous shells. It shows what the *Rmerge* would be if the data is cut off at different I/σ levels.

Remark: Use the table to determine at what resolution the crystal stopped diffracting.

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```
270 Rmerge vs Resolution
271 ------------------------------------------------------------------------------
272 Resolution Average Num Num Num Num <I/ ChiSq Rmerge Rmerge
273 range counts obs rejs ovlps mults sig> norm shell cumul
274 ------------------------------------------------------------------------------
275 79.2 - 6.12 2260 278 31 228 64 21.2 0.797 0.042 0.042
276 6.12 - 4.34 2346 1564 44 1468 351 28.2 0.945 0.029 0.031
277 4.34 - 3.54 3147 2196 37 2095 492 33.7 0.934 0.024 0.027
278 3.54 - 3.07 2102 2586 39 2482 603 32.0 1.014 0.026 0.026
279 3.07 - 2.74 1055 2963 55 2836 705 27.5 1.086 0.030 0.027
280 2.74 - 2.51 597 3137 69 2982 747 22.7 1.125 0.036 0.028
281 2.51 - 2.32 382 3321 74 3170 834 17.6 0.999 0.045 0.029
282 2.32 - 2.17 278 3378 76 3199 832 14.0 1.028 0.057 0.030
283 2.17 - 2.05 192 3204 72 3002 813 11.0 0.999 0.071 0.031
284 2.05 - 1.94 118 3993 88 3676 1049 8.4 0.890 0.090 0.032
285 ------------------------------------------------------------------------------
286 79.2 - 1.94 941 26620 585 25138 6490 19.5 1.00 0.032 0.032
```

Lines 270-286 This table lists Rmerge vs Resolution

`Resolution range` The resolution range of the shell in Ångstroms.

`Average counts` The average counts of reflections in the shell. This includes reflections that overlap and those that do not. If you assume Poissonian counting statistics, then the expected *Rmerge* for this shell would be $1/I$. So for the shell of highest I/σ, $1/2260 = 0.021$ which is inconsistent with 0.042 found. It was then discovered that low resolution reflections which were obscured by the asymmetric beamstop were not rejected, hence the higher *Rmerge* for this shell. In the 2.05-1.94 shell, $1/118 = 0.092$ is consistent with 0.090 found.

`Num obs` Number of reflections in this shell.

`Num rejs` Number of rejected reflections. There should be very few, if any rejected reflections. Any shell with a large number of

rejected reflections should be investigated. Perhaps the shell contains extraneous diffraction from ice.

`Num ovlps` Number of reflections in this shell having symmetry-related mates and that contributed to the *Rmerge*.

`Num mults` Number of unique reflections measured multiple times in the shell. The average multiplicity or redundancy for the shell is `Num ovlps / Num mults`.

`<I/sig>` The average Intensity/SigmaI for averaged reflections in the shell. As expected, there is a larger `<I/sig>` for the averaged reflections than shown for unaveraged reflections in the *Rmerge vs Batch* table.

`ChiSq norm` This is the normalized χ^2 popularized by Dr. Zbyszek Otwinowski. Values close to 1 suggest that the error model is valid.

`Rmerge shell` This is the *Rmerge* for reflections which belong to this shell.

`Rmerge cumul` This is the cumulative *Rmerge* for reflections which belong to this shell and all previous shells. It shows what the *Rmerge* would be if the data were cut off at different resolution levels.

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```
287 Completeness vs Resolution
288 ------------------------------------------------------------------------------
289 Resolution Calc Num Num Num Num Num Avg %Comp %Comp
290 range unique obs rejs mults single unique mult shell cumul
291 ------------------------------------------------------------------------------
292 79.2 - 6.12 363 278 31 64 19 83 2.98 22.9 22.9
293 6.12 - 4.34 593 1564 44 351 52 403 3.77 68.0 50.8
294 4.34 - 3.54 736 2196 37 492 64 556 3.88 75.5 61.6
295 3.54 - 3.07 863 2586 39 603 65 668 3.81 77.4 66.9
296 3.07 - 2.74 966 2963 55 705 72 777 3.74 80.4 70.6
297 2.74 - 2.51 1061 3137 69 747 86 833 3.68 78.5 72.5
298 2.51 - 2.32 1131 3321 74 834 77 911 3.56 80.5 74.1
299 2.32 - 2.17 1226 3378 76 832 103 935 3.53 76.3 74.4
300 2.17 - 2.05 1290 3204 72 813 130 943 3.32 73.1 74.2
301 2.05 - 1.94 1362 3993 88 1049 229 1278 3.06 93.8 77.0
302 ------------------------------------------------------------------------------
303 79.2 - 1.94 9591 26620 585 6490 897 7387 3.52 77.0 77.0
```

Lines 287-303 This table lists *Completeness vs Resolution*. In order to perform subsequent crystallographic analyses, you would like to have very complete data.

`Resolution range`The resolution range of the shell in Ångstroms.

`Calc unique` Number of calculated unique reflections in this shell. This is calculated from the unit cell dimensions and the space group in an exact manner (it is not an approximation).

`Num obs` Number of observations for reflections in this shell. The more the better.

`Num rejs` Number of rejected reflections. There should be very few, if any rejected reflections. Any shell with a large number of rejected reflections should be investigated. Perhaps the shell contains extraneous diffraction from ice or low resolution reflections are behind the beamstop. (Notice that more than 10% of the observations in the lowest shell are rejected. That's bad!)

`Num mults` Number of unique reflections resulting from the overlaps in the shell. In other words, the number of unique reflections measured more than once.

`Num single` Number of unique reflections measured just once.

`Num unique` Number of unique reflections measured (`Num mults + Num single`).

`Avg mult` The average multiplicity or redundancy in the reflections in the shell. Simply `(Num obs - Num rejs) / Num unique`.

`%Comp shell` This is the percent completeness for reflections which belong to this resolution shell: `100 x Num unique / Calc unique`.

`%Comp cumul` This is the cumulative percent completeness for reflections which belong to this shell and all previous shells. It shows what the completeness would be if the data were cut off at different resolution levels.

Direct Beam Log

A summary of the typical log file `DirectBeam.log` generated by the direct beam shot utility is shown below.

```
1 Direct Beam Utility Copyright (c) 1998 Molecular Structure
Corporation
2 Number of cycles: 5
3 Exposure time: 1 seconds
4 Date: Thu Mar 30 16:41:19 2000
5 ....................
6 ....................
7 ....................
8 .......111111........
9 ......111111111......
10 .....11122222111.....
11 ....112233333211.....
12 ...11123456543211....
13 ..11223579A9753211...
14 ..112357ADFFB85311...
15 .112357AFJNMHB6321... Direct beam for IP 1, cycle 1
16 .112469DJQUTNE8421... Position (x,y) = (1499.84, 1509.80)
17 .11247AFMUZXQG95211.. Pixel Intensity = 10841
18 .11247BGOV+YQG9521... Integrated Intensity, sigma(I) = 330647,
895
19 .11246AGMTXVNF8421... I/sigma(I) = 369.5
20 ..12358DIORQKC7321... 3sigma width (x,y) = (12, 13)
21 ..112469DHJJE95311... Full width at half maximum (x,y) = (5.57,
6.86)
22 ...123469BDDA7421....
23 ...11234578875321....
```

```
24 ....1122345553211....
25 ....111223333211.....
26 .....11111222111.....
27 .......11111111......
28 .........11111.......
29 ......................
30 ......................
31 ......................
32 ...
33 Average direct beam results for IP 1
34 Position (x,y) = (1499.64, 1509.61) +/- (0.262854, 0.14148)
35 Pixel Intensity = 10533 +/- 445.806
36 Integrated Intensity, sigma(I) = 336594, 893.455 +/- (4324.93,
4.73774)
37 I/sigma(I) = 376.732 +/- 4.30341
38 Full width at half maximum (x,y) = (5.55258, 6.88398) +/-
(0.0486711, 0.0397825)
```

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```
39 Average direct beam results for IP 2
40 Position (x,y) = (1500.92, 1509.61) +/- (0.266244, 0.175193)
41 Pixel Intensity = 10740.4 +/- 268.098
42 Integrated Intensity, sigma(I) = 336789, 896.288 +/- (4495.92,
3.81553)
43 I/sigma(I) = 375.777 +/- 6.19005
44 Full width at half maximum (x,y) = (5.57419, 6.89354) +/-
(0.0479199, 0.0299656)
45 IP1 IP2
46 Cycle x y I x y I
47 ----- ---------------------- ----------------------
48 1 1499.8, 1509.8 [ 10841] 1500.7, 1509.8 [ 10932]
49 2 1499.4, 1509.6 [ 10346] 1501.3, 1509.4 [ 10267]
50 3 1499.4, 1509.4 [ 9872] 1501.0, 1509.7 [ 10826]
51 4 1499.6, 1509.7 [ 11006] 1500.9, 1509.5 [ 10846]
52 5 1500.0, 1509.5 [ 10600] 1500.7, 1509.6 [ 10831]
```

Lines 5-31 ASCII text representation of the spot profile. Each character represents the value of a pixel. Pixel values are on a 0-35 scale (0 is represented by ., 10-35 are represented by A-Z). Pixel closest to the center of the spot is represented by a +.

Line 15 For R-AXIS systems, the IP number and cycle number are listed. For CCD systems, a description of the type of CCD is listed.

Lines 16-17 The position of the center of the spot and the value of the pixel closest to the center are listed.

Lines 18-19 The integrated intensity, I, $\sigma(I)$, and $I/\sigma(I)$ for the peak are listed.

Lines 20-21 The width of the peak, at the 3σ level and at half of the maximum value of the peak are listed.

Lines 33-38 For R-AXIS systems, the results for IP1, averaged over all of the cycles. For CCD systems, these lines do not appear in the file.

Lines 39-44 For R-AXIS systems, the results for IP2, averaged over all of the cycles. For CCD systems, these lines do not appear in the file.

Lines 48-52 For R-AXIS systems, the direct beam positions and pixel value tabulated for each IP and cycle. For CCD systems, these lines do not appear in the file.
Important: If either X-beam or Y-beam position differ from IP1 or IP2, this will be corrected at the time of data collection using the values from the direct beam shots. If the values of either X-beam position differs on the same IP between cycles, the adjustments may be needed for the IP belt itself.
A summary of the typical summary file `DirectBeamSummary.log` generated by the direct beam
shot utility is shown below.

```
1 Direct Beam Utility
2 Number of cycles: 1
3 Exposure time: 1.0 seconds
4 Date: Thu Sep 30 17:34:19 1999
5 Average direct beam position for IP1 = (2682.6,1505.9)
6 Average direct beam position for IP2 = (2683.5,1505.5)
7 IP1 IP2
8 Cycle x y I x y I
```



```
9 ----- ---------------------- ----------------------
10 1 2682.6, 1505.9 [ 7090] 2683.5, 1505.5 [ 7209]
11 Direct Beam Utility
12 Number of cycles: 2
13 Exposure time: 1.0 seconds
14 Date: Tue Oct 19 11:02:31 1999
15 Average direct beam position for IP1 = (1505.1,1506.6)
16 Average direct beam position for IP2 = (1507.1,1506.7)
17 IP1 IP2
18 Cycle x y I x y I
19 ----- ---------------------- ----------------------
20 1 1504.2, 1507.0 [241280] 1506.2, 1506.8 [247008]
21 2 1506.1, 1506.3 [ 14490] 1508.0, 1506.7 [ 14340]
22 ...
23 Direct Beam Utility
24 Number of cycles: 5
25 Exposure time: 1.0 seconds
26 Date: Thu Mar 30 16:56:17 2000
27 Average direct beam position for IP1 = (1499.6,1509.6)
28 Average direct beam position for IP2 = (1500.9,1509.6)
29 IP1 IP2
30 Cycle x y I x y I
31 ----- ---------------------- ----------------------
32 1 1499.8, 1509.8 [ 10841] 1500.7, 1509.8 [ 10932]
33 2 1499.4, 1509.6 [ 10346] 1501.3, 1509.4 [ 10267]
34 3 1499.4, 1509.4 [ 9872] 1501.0, 1509.7 [ 10826]
35 4 1499.6, 1509.7 [ 11006] 1500.9, 1509.5 [ 10846]
36 5 1500.0, 1509.5 [ 10600] 1500.7, 1509.6 [ 10831]
```

Lines 1-10 Summary of direct beam shots taken on 30 September 1999
Lines 11-21 Summary of direct beam shots taken on 19 October 1999
Lines 23-36 Summary of direct beam shots taken on 30 March 2000

Important: If either X-beam or Y-beam position differ from IP1 or IP2, this will be corrected at the time of data collection using the values from the direct beam shots. If the values of either X-beam position differs on the same IP between cycles, the adjustments may be needed for the IP belt itself

PMTCheck Log

A summary of the typical log file `PMTCheck.log` generated by the PMT check utility is shown below.

```
1 PMT Check Utility Copyright (c) 1998,1999 Molecular Structure
Corporation
2 Date: Wed Apr 05 15:52:11 2000
```



```
3 Result of PMT Test:
4 Average = 5.5770
5 3*Sigma = 1.8184
6 Number of 0 pixels = 0/252000
```

Line 4: The average background counts in the image.
Line 5: The 3σ level of the background.
Line 6: The number of pixels in the image with a value of 0.

A summary of the typical log file `PMTCheckSummary.log` generated by the PMT check utility is shown below.

```
1 PMT Check Utility
2 Date: Wed Jan 05 12:21:51 2000
3 Result of PMT Test:
4 Average = 6.354
5 3*Sigma = 1.623
6 Number of 0 pixels = 0/252000
7 PMT Check Utility
8 Date: Wed Apr 05 15:52:11 2000
9 Result of PMT Test:
10 Average = 5.5770
11 3*Sigma = 1.8184
12 Number of 0 pixels = 0/252000
```

Lines 1-6: Results of the PMT check run on 05 Jan 2000.
Lines 7-12: Results of the PMT check run on 05 April 2000.

Continuous IP Read Log

A summary of the typical log file `ContinuousIPRead.log` generated by the PMT check utility is
shown below.

```
1 Continuous IP Read Utility Copyright (c) 1998 Molecular Structure
Corporation
2 Date: Thu Feb 10 12:19:01 2000
3 Continuous IP Read test[1/100] => OK Error count = 0
4 Continuous IP Read test[2/100] => OK Error count = 0
5 Continuous IP Read test[3/100] => OK Error count = 0
6 Continuous IP Read test[4/100] => OK Error count = 0
…
7 Continuous IP Read test[100/100] => OK Error count = 0
8 Results of Continuous IP Read test:
```

```
9 Number of Read Write Other Total
10 Cycles Failures Failures Failures Failures
11 100 0 0 0 0
```
Lines 3-7: Success/Failure results of the IP reads.
Lines 8-11: Summary of the number of cycles performed and the number and types of errors encountered.
A summary of the typical log file `ContinuousIPReadSummary.log` generated by the PMT check
utility is shown below.
```
1 Continuous IP Read Utility
2 Date: Thu Oct 07 11:51:04 1999
3 Results of Continuous IP Read test:
4 Number of Read Write Other Total
5 Cycles Failures Failures Failures Failures
6 5 1 0 0 0
7 Continuous IP Read Utility
8 Date: Thu Feb 10 12:19:01 2000
9 Results of Continuous IP Read test:
10 Number of Read Write Other Total
11 Cycles Failures Failures Failures Failures
12 100 0 0 0 0
```
Lines 1-6: Summary of the IP reads done on 07 October 1999.
Lines 7-12: Summary of the IP reads done on 10 February 2000.

Appendix D: Troubleshooting
This section covers a few common problems that you may encounter in *CrystalClear*, how you can solve
those problems.
General CrystalClear Problems
Problem Solution
CrystalClear does not
communicate correctly with the
X-ray detector on a Windows
95 machine.
CrystalClear uses Windows Sockets to communicate with the X-ray detector and with compute server modules. While Windows NT includes the Windows Sockets module, Windows 95 does not. Install the Winsock module, WS295SDK.EXE, which is located in the *CrystalClear* directory.
Make sure the detector is set up correctly.
When I start *CrystalClear*, only
the menus are displayed. I do
not see a full *CrystalClear*
window – only the task bar.
CrystalClear was closed while it was minimized. After logging into

CrystalClear and selecting the project/sample, right-click *CrystalClear* on the task bar and select **Maximize**. Close CrystalClear while it is maximized. Open *CrystalClear* and log in. Now you can reshape the *CrystalClear* window.

You attempt to select a processing algorithm, such as d*TREK, PROCESS, or TwinSolve, and you receive the following message: "You must have a sample open to set processing algorithms."

You must have a sample open before you can select a processing algorithm. Click **File > Open Sample** from the menu to select a sample, or **File > New Sample** to create a new sample.

The TwinSolve button is grayed out on the Toolbar.

TwinSolve is only available with the Mercury CCD.

You wish to process data, but the selections on the flow bar do not include processing options.

You have a Collection task selected. From the Task drop down, select a task that includes processing, such as the Process task.

The settings shown in a dialog have reverted back to the defaults, instead of to settings you specified in a previous session.

Your previous settings were not saved. Specify the desired settings, then click the Save button on the dialog. Specify the location to save the settings to, and click OK.

CrystalClear takes a long time to respond, then an error message occurs saying that *CrystalClear* cannot get a response from the RAXIS.

If you are not actually connected to an X-ray detector, you should make sure *CrystalClear* is set in Simulator mode. Click **Tools > Preferences**, then click the Server tab. Check the detector in the list to force *CrystalClear* to run in Simulator mode.

When you attempt a step that requires communication with the CCD Camera, CrystalClear

Open system.configuration, which is found in the *CrystalClear* directory, and change the value of "DaemonIP" to be the IP address of the computer on which the Rigaku Daemon is running. 9 This solution

hangs. applies if MSCServDetCCD.exe or MSCServDetCCD_Simulator.exe

is started before the hang occurs.
You installed *CrystalClear* 1.2
over a 1.1 version, and now
your user list is empty.
Your data is not removed when you uninstall or reinstall, so you can just recreate the users in *CrystalClear*, making sure you use the same names as the previous version.
In the User Settings screen for each user, specify the path to the user's directory in the **Data** field.
You receive an error when
attempting to run CrystalClear:
"A required DLL file
WS2_32.DLL was not found."
This error will occur on Windows 95 machines if Winsock has not been installed. The Winsock installation file is included in this installation. To install Winsock2, go to the *CrystalClear* directory after this installation (usually c:\Program Files\Rigaku MSC\CrystalClear) and run WS295SDK.EXE. This will copy the Winsock setup files to your hard drive.
Next, run the Winsock setup by going to the Winsock directory (usually c:\ws295sdk\setup) and run Ws2setup.exe.

Crypto-Box Messages

Problem Solution

Crypto-Box Error 8: no dongle
found.
The *CrystalClear* Crypto-Box dongle was not found. Install the dongle and try again.
Crypto-Box Error 30: Error, the
attached Crypto-Box did not
come from MSC.
A Crypto-Box was found but it was not issued by MSC. The dongle that came with *CrystalClear* should be installed on the PC on which *CrystalClear* is installed.
Crypto-Box Error 31: Error,
registration key in the registry
and registration key in the
Crypto-Box do not match.
Normally this is caused when *CrystalClear* was installed with an incorrect license number. In this case, reinstall *CrystalClear* and input the correct license number during installation.
This error can also occur if a non-*CrystalClear* Crypto-Box dongle is found on the PC, but the *CrystalClear* dongle was not. In this case, install the *CrystalClear* Crypto-Box and *Crypto-Serv* software on the PC, then click the **Check Again** button.

Appendix E: Absorption in Scaling

CrystalClear provides a number of options for the modeling of absorption, crystal decay and incident beam intensity drift. These are all modeled within the absorption correction algorithms provided in the Scaling and Averaging step.

The goal of the absorption correction algorithm is to deduce an absorption surface associated with a crystal by requiring that this surface minimize the difference in intensities between symmetry related reflections. In practice, this is done by minimizing the weighted differences between the right and lefthand
sides of the equation:

(1)

where I's are the intensities and *A*'s are the absorbances. The right hand side represents a sum over the k
symmetry related intensities in a group of equivalent reflections, and the subscript i represents any member in the group. One seeks to find an absorbance A_i to minimize this difference and A_j $_0$ represents
an initial estimate of the absorbance. As implemented in the program the initial A_0 values correspond to
that of the spherical crystal; when a new absorption surface is obtained, these replace the original A_0 values and the process is repeated until convergence is obtained.

The absorbance *A* consist of a product of the absorbance of the primary beam and the absorbance of the
scattered beam, i.e.

(2)

These absorbances could also be expanded in a Taylor series,

(3)

If the usual approximation is made of assuming that the higher order contributions are negligible, then by
a least squares approach, the Δp_j values can be calculated and the whole process repeated until convergence is obtained. We assume the absorption surface is smoothly varying in reciprocal space. In
order to enforce this powerful constraint two sets of analytical functions are used.

Spherical harmonics[1] are one convenient set of analytic functions for A_s. The maximum order is limited to 8, four even term and four odd terms:

(4)

[1] Blessing, R. H. (1995). *Acta Cryst*. A**51**, 33-38.

$$\sum$$

$$\sum$$

$$= = k$$

$$j$$

$$j$$

$$k$$

$$j$$

$$j\,j\,j$$

$$i\,i$$

$$w$$

$$w\,I\,A$$

$$I\,A\,1$$

$$0$$

$$p\,s$$

$$A = e\,_t = e\,_{t\,p\,ts} = A \cdot A\,_{-u\,-u\,(+)}$$

$$\Delta + \text{higher order terms}$$

$$\partial$$

$$\partial$$

$= + \sum_{j}$
$j\, j$
$_{o}\, p$
p
A
$A\, A$
$(,) (,)$
0
8
1
$f\, u\ _{0\ lm\ lm}\, f\, u$
l
m
l
l
$A\ a \sum \sum a\ y$
$=$
$\leq$
$=$
$= +$

Appendix E: Absorption in Scaling

where a_{lm} represents the coefficients to be determined by refinement and y_{lm} are the corresponding spherical harmonics, and φ and υ are the equatorial and azimuthal angles of the diffracted x-ray beam,
respectively.

An alternate analytic function employs a Fourier series to represent absorbance:[2]
(5)

Here the coefficients P_{nm} and Q_{nm} are fit via a least squares procedure. The maximum values of *n* and *m*
are 8 and 4, respectively. In this case of the Fourier method both the primary (or incident) and scattered
beams are modeled.

In addition to absorption, the apparent intensity of the primary or incident beam may be affected by decay, beam in homogeneity and source instability. CrystalClear provides two methods for modeling these effects, simple batch scaling, which is applicable to either the spherical harmonics and Fourier methods, and circular harmonics, which applicable to only with only the spherical harmonics.

In the batch scaling method the data are first scanned to find the batch with the greatest overlap. This batch becomes the reference batch and the absorbances described in Equation 3 are allowed to vary with
respect to the reference batch. That is, the derivatives $\partial A/\partial p_j$ are zero unless j corresponds to a batch and
the reference batch.

Alternatively, if the azimuthal angle in equation 4 is fixed at 0, the spherical harmonics collapse into the
equatorial plane becoming circular harmonics and the resulting function *A(f,0)* can be used to model incident beam absorption[3].

CrystalClear provides nine options for scaling and absorption correction. The options are found in the Scaling and Averaging Dialog and are described in Table 1. The option "4th 3D + 4th 2D" appears to be

the most robust and effective for small molecule data. However, “Fourier and batch” is the best method
for macromolecule data. The preceding statements are generalizations. If one method does not provide the
results you were expecting try one of the other methods. You will find this useful in special cases.
Fitting the absorption surface using spherical harmonic coefficients or Fourier coefficients via singular
value decomposition[4] is very robust and, in most cases, will lead to a satisfactory result. However, there
are some cases in which error messages are displayed. Use the troubleshooting tips in Table 2 to guide
yourself through these problem cases.

[2] Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158.

[3] Jacobson, R. A., private communication.

[4] Press, W. H., Flannery, B. P., Teukolsky, S. A., Vetterling, W. T., *Numerical Recipes in C: The Art of Scientific Computing*, Cambridge University Press, Cambridge, **1991**, pps. 60-72.

(cos( ) cos( ))

(, , , (sin( ) sin( ))

max max

0

nm p p s s

nm p p s s

n m

p s p s

Q n m n m

A Q P n m n m

n m

f u f u

f f u u f u f u

+ + + +

= + ∑ ∑ + + + +

Appendix E: Absorption in Scaling

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Table 1. Absorption options

Fourier This option uses Fourier coefficients to model diffracted beam absorption and simple batch scaling to model incident beam absorption, decay, etc.

4th 3D + 3rd 2D This option uses 4th order even and odd spherical harmonics to describe the diffracted beam absorption and 3rd order even and odd circular harmonics to model incident beam absorption.

3rd 3D + 2nd 2D This option uses 3rd order even and odd spherical harmonics to describe the diffracted beam absorption and 2nd order even and odd circular harmonics to model incident beam absorption

Table 2. Absorption correction trouble shooting guide.

Error Message	Cause and remedy
Number of outliers exceeds 2000	1. The assumed symmetry is too high. Use “Data analysis -> Laue Group” to automatically determine the Laue group and rerun. 2. The sample is a strong absorber, μR > 2. In the Advanced

Menu set outlier rejection criterion to 500 or 1000. This will ensure reflections that are strongly affected by absorption will be used in the calculation of the surface improving the overall correction.
3. The crystal is split and some reflections overlap and some do not. Try to find a better crystal.
No convergence in SVDCMP 1. The redundancy is low. If the sample is triclinic try to collect at least one scan of 180º. If the sample is of higher symmetry collect more data in a different region of f or ?.
2. The diffraction data are poor. The algorithms significant data to calculate the absorption surface reliably and there are not enough to do this. Recollect the data with longer exposure times.
Spherical harmonics methods do not complete
`S Del**2` > 10_6
1. Multiple scans have different exposure times. You may be able to recover by repeated runs of "Fourier".
2. The crystal died or fell off, the generator went down, etc. Inspect your images to determine if diffraction stopped at some definite point in time and reintegrate up to that point.
3. The assumed symmetry is too high. Change the putative space group.
Fourier methods do not complete.
`S Del**2` > 10_6
1. Multiple scans have different exposure times. Recovery unlikely.
2. The crystal died or fell off, the generator went down, etc. Inspect your images to determine if diffraction stopped at some definite point in time and reintegrate up to that point.
3. The assumed symmetry is too high. Change the putative space group

Appendix F: Defaults in CrystalClear

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Appendix F: Defaults in CrystalClear

New Sample Defaults

When a new sample is created, the defaults are obtained from the project under which it is created.
Example: When sample `Zn_13` was created, a copy of the defaults from project `Zn` was made and assigned to `Zn_13`.

Inherited Defaults

When the user saves defaults at the project level, the changes are *not* automatically reflected in other, existing samples in the project. However, any new samples created will reflect the changes.
Example: If the user changes defaults in `Zn_13` and then saves to the project level, `Zn_cub` will *not* be modified as a

result. Thus: Zn_13 = Zn ≠ Zn_cub. If the user creates a new sample Zn_14, its defaults will be identical to Zn. Thus: Zn_13 = Zn_14 = Zn ≠ Zn_cub.
When the user saves defaults at *all* levels, the defaults are only immediately reflected in objects residing
in a direct line from the sample currently open to the site level. **Example**: If the user changes defaults in
May22a and then saves to all levels, the defaults will be reflected in the following databases:

- May22a (Sample)
- May22 (Project)
- mdavis (User)
- Site

The new defaults are not immediately reflected in any other object. May22b, Myo1, sgrapelli,
… all remain the same. If a new user cparker is then added it will receive its new user defaults from
Site Level
User Level
Project Level
Site
pwoods mdavis sgrapelli
Zn Myo1 May22 Cyt
Zn_13 Zn_cub
Myo1_3
May22a May22b Cyt_try1
Sample Level

Appendix F: Defaults in CrystalClear

the site level. However, if pwoods adds a new project Abt it will *not* reflect the site-level changes because new projects obtain their defaults from the user level, and pwoods does not yet reflect the sitelevel
changes.

Updating Defaults

One difficulty is that the user may want changes to the site level reflected in all other users. The way to
do this is to have each user log in and open a sample. They should then load the site-level defaults and
save defaults to the user level. **Example**: mdavis changes May22b and saves defaults to all levels. If
pwoods then logs onto CrystalClear and opens sample Zn_13. She then loads the site-level defaults
into the sample, and then saves defaults to the project and user level. Now any new project she makes will inherit the defaults she just saves at the user level. In addition, any new sample she creates (unless it
is created in some already existing project that isn't Zn) will have these new defaults.
Note: *CrystalClear* 1.2.x allows only the administrator to save defaults at the user and site levels. *CrystalClear* 1.3 allows any user to save up to the user level. Administrator privileges are required only

for saving at the site level.

Dialog Defaults

RAXIS Jupiter Mercury

Setup

Crystal To Detector
Distance
120 80 50
2-theta 0 0 0
Crystal 1 unit cell 80 90 100 90 90 90 80 90 100 90 90 90 10 10 10 90 90 90
Crystal size 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2
Mosaicity 0.6 0.6 0.6
Color Colorless Colorless Colorless
Mount Loop Loop Fiber
Morphology Prism Prism Prism
Crystal 2 Unknown Unknown Unknown
Orientation 0 0 0 0 0 0 0 0 0
Detector Translation 0 0 120 0 0 120 0 0 50
Rotations 0 0 0 0 0 0 0 0 0
X-ray Source 50kV 100mA 50kV 100mA 50mV 40mA
Copper 1.5418 Copper 1.5418 Molybdenum
0.71073
Source Rotating anode Rotating anode Sealed Tube
Optics Confocal Confocal Graphite
monochromator
Focus 0.3 0.3 1.0
Collimator 0.3 0.3 0.5

Initial images

Images 1 scan of 2 images at 1 scan of 2 images at 4 scans of 1 image at

Appendix F: Defaults in CrystalClear

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0, 90 degrees 0, 90 degrees 0, 30, 60, 90 degrees
Readout Full frames
Exposure 2 min/image 2 min/image 5 sec/image
Pixel resolution 100 um pixel 2x2 binned 2x2 binned

Find

Images First image of screen 1-2 of screen 1-4 of screen
1-100 if already
collected
I/sigma level 3 sigma 3 sigma 3 sigma
Min pixel 50 50 20
Peak filter 6 6 6
Box 0 0 0 0 0 0
2D/3D 2D 2D 3D
Resolution 0 0 0 0 0 0

Index

Known cell? Unknown Unknown Unknown
User chooses solution Yes yes yes
Reflection file dtfind.ref dtfind.ref dtfind.ref

Max residual 3 3 3
Indexing method 1D FFT 1D FFT 1D FFT

Refine

Resolution limits 0 0 0 0 0 0
Cycles 100 100 100
I/sig 0 0 4
Rejection limits 1 1 2 1 1 2 1 1 2
Macro All all All

Predict

Images First image of first
scan, screen images
unless collect images
are available
1-10 of collected
images
1-10 of collected
images
Mosaicity 0.6 unless refined 0.6 unless refined 0.6 unless refined

Strategy

Per cent
completeness
99
Resolution 0 0
Speed Very fast
Result Limit 360
Search Rotation 0 360

Collect

Exposure time 2 min RAXISIV++
4 min RAXIS IV
8 min RAXIS II
10-20 sec, sample
dependant
20-30 sec, sample
dependant
Pixel resolution 100 um pixel 2x2 binned 2x2 binned
Readout Full

Integration

Images All collection images All collection images All collection images

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Images per batch 4 4 10
Padding 1 1 2
Pre-refinement 5 5 5
Resolution 0 0 0 0 0 0
Box 0 0, user sets 0 0, user sets 0 0, user sets
Refinement macro All All All
Peak radius min/max 3/0 3/0 2/0

Laue

Reflection file dtprofit.ref Dtprofit.ref dtintegrate.ref
Residual 0.15 0.15 0.15

Centricity

Reflection file dtprofit.ref Dtprofit.ref dtintegrate.ref

Spacegroup

Reflection file dtprofit.ref Dtprofit.ref dtintegrate.ref
I/sig 4 4 10

Scale and Average

Reflection file dtprofit.ref dtprofit.ref dtintegrate.ref
Algorithms Batch, absorption Batch, absorption Batch, absorption
Absorption Spherical 4,3 Spherical 4,3 Spherical 4,3
Exclude sigma 3 3 3
Error model mul Auto-intelligent Auto-intelligent 2.5
Addend Auto-Rmerge Auto-Rmerge Auto-Rmerge
Rejection sigma 50 50 10
Chi square Max fraction 0.0075 Max fraction 0.0075 Max fraction 0.0075
Scale anomalous No No No
Optional output Output anomalous Output anomalous Uncorrected, unaveraged
Output name F2plus.dat
Resolution 0 0 0 0 0 0

Appendix F: Defaults in CrystalClear

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Using the Default Manager

The **Default Manager** dialog allows you to save at the **User Level**, **Project Level**, or **Sample Level**. Using **Default Manager** also allows you to make information available to other samples or all projects, in other projects and samples. **Site Level** settings are inherited by all users for each project and sample, as they are created. Only users with "*administrator*"' privileges are authorized to save at **Site Levels**. For most users, this option is grayed-out.

- *To access "administrator" privileges, exit **CrystalClear** and log in as an administrator.*
- *If a user wishes to access the **Site Level**, "administrator" privileges may be assigned" in the **User Settings** dialog .*

For more information, see Edit User Settings *on page 145 of* Appendix B: Administration.

1. When the **Default Manager** dialog appears, select the **Current Levels** you wish to save by clicking the appropriate check box.

- *Alternatively, selections can be made by clicking the radio-button beside the appropriate Site, User, Project, or Sample names (on right side of dialog).*

2. Use the following buttons for assistance in setting defaults:

- **Set** Sets a default
- **Unset** Unsets a default
- **Set All** Sets all Levels
- **Unset All** Unsets all Levels

3. When appropriate **Levels** are selected, click **OK**.

Appendix G: Crystallographic Troubleshooting

This section covers a few common crystallographic problems that you may encounter in *CrystalClear*,
and how you may solve those problems.

Problem Solution

The crystal to detector distance is not editable…it states "Per Scan"

In this sample there are images with different crystal to detector distances. Try looking in the Scan State Display for information relative to each scan.

I started a sample as a Process task and the crystal to detector distance shows "0".

You collected the data without setting the crystal to detector distance in the software for addition into the header. If you know what the distance is, edit the field in the Setup dialog and continue. If you do not know what the true crystal to detector distance is, try:

1. In an image display window, turn on the arcs tool and play with the crystal to detector distance in the image information area. The arcs will change size and shape relative to this (and the 2-theta angle). See if you can line up a ring (ice, salt, etc.). Then take these numbers to the Setup dialog and edit the fields.
2. Set a best guess in the crystal to detector distance field in Setup and try to index. The closer you are to the read crystal to detector distance (or any geometric parameter), the lower the residual of the correct lattice. This may be quite a bit of work. If no solutions pop out after many attempts, Find Peaks off 2 (or more) images in the same scan separated by nearly 90 degrees and use difference vectors in indexing.
3. If the lattice is uncertain, but the detector parameters are remembered vaguely, try indexing and using the triclinic cell for refinement…then reindex to see if the higher symmetry cell is determined.

How do I change the resolution ranges for all steps in processing

Anywhere there are Resolution Limits fields and a "Set" box, select the box and choose the processing steps to use the resolution limits currently in the edit fields and press "OK".

You have no idea what the cell lengths may be.

In an image display window zoom in on an area where spots are regularly spaced. Turn on the measure tool by selecting the ruler icon. Touch on one spot and drag to an adjacent spot. The inter-spot distance will be displayed as you drag.

The red plus sign is not in the

beam stop shadow
You are collecting images with an improper direct beam position and should contact your administrator to redo direct beam shots
I got the “Find Spots Failed” message and the log file shows
“...reading image lys0001.osc...
Error opening file lys0001.osc
Error is: -2”
The image is not there or is corrupted. Wait for the image read to finish.
Find only found a few spots. 1. Decrease the I/sigma
2. Widen the resolution range
3. Decrease the minimum pixel value
4. Decrease the peak filter.
Find Spots found too many reflections.
1. Slide the number of spots slide in the image information window

reflections. 2. Use the delete spots icon to delete spots.
3. Set the I/sigma higher in Find Spots
There are lots of spots very close to each other.
Increase the box size.
Indexing is incorrect based on the measure tool distances.
1. Check that the crystal to detector distance, X and Y beam positions, wavelength, and 2-theta angle are correct.
2. Indexing may be correct if there is additional symmetry…continue on to prediction for varification.
3. If the peak shapes are poor, then try raising the I/sigma level to avoid the weaker peaks. Additionally, this will likely force the larger twin portion to index.
4. If the cells are all much too large, including the triclinic, set the maximum cell in the indexing to a smaller value (about 2x that of the closest spot separation for starters).
I don’t see all the crystal lattices in the table of indexed lattices
Set the maximum residual in the advanced tab of index to 100.
The software keeps choosing the wrong lattice in indexing
Use the “User Chooses Solution” option in index. Upon completion, choose the lattice from the list. If all the lattices are not displayed, increase the maximum residual.
Few of the reflections are included during refine.
Adjust the resolution limits, I/sigma, and rejection limits.
The “test mosaicity” is greyed

out
You are using “Reflection List” to “Refine on”. Set this to “Images” and edit the “To Use” field. A range of images must be used for this refinement.
There is no reflection file list in the refine dialog
You are using “images” to “Refine on”. Set this to “Reflection List”
All of the option boxes are greyed out in the refine dialog
You are using the “All” macro. Select “Single Step Refine” to toggle on/off individual parameters.
There are more/less spots than prediction circles on my predicted image.
In the Predict Spots dialog increase/decrease the mosaicity and predict again. Or, you may have the wrong cell and need to reindex.
The predictions are terribly wrong and I wish to start from scratch with the images again
Open the Processing State Display, go to the State History, press the down arrow, scroll to the bottom, select one of the earlier states (like “1. Setup” or “2. Find Run”) and “Set as current”
Refinement seems to have stopped during integration.
Try increasing the number of images per batch.
I don’t want to refine mosaicity during integration.
Return to the refine dialog, set a value in the mosaicity field, and uncheck the mosaicity box. Go back to integration and restart.
Can I get rid of ice rings during integration?
Sure. Go to the advanced tab of Integrate Reflections and Add/Delete rings to the list (avoided area in integration).
Integration keeps stopping when it finishes all the images on disk at the time and I want it to wait for the images to appear.
Adjust the wait limit in the Advanced tab of Integrate Reflections. If an image is not on disk when integration gets to that image, it will query the disk every 15 seconds until it either finds the image (integrates and looks for the next image) or reaches the end of the wait limit (completes integration with the reflections it has to that point)
What should I do if Laue shows that I integrated the data in the wrong crystal system.
Here you will need to think about what it is showing you. In general, if the symmetry during integration is higher than merited by Laue, then you should consider reintegrating. If the symmetry is higher than that for integration, it is recommended that you reintegrate, but you may

Appendix G: Crystallographic Troubleshooting

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still have good data which is usable for a first reflection file.
I need to have a different format
for my reflection file.
In the CCP4 suite there is a conversion program to convert to mtz
format from the d*TREK format.

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