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 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.
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 $\chi^2$ 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.
# Table of Contents

CRYS\L\ALCLEAR USER’S MANUAL (ABRIDGED) ................................................................. 3

CRYS\L\ALCLEAR USER’S MANUAL (ABRIDGED) ................................................................. 5

TABLE OF CONTENTS ........................................................................................................ 7

1 ABOUT THIS MANUAL ...................................................................................................... 11

WHAT YOU SHOULD KNOW .......................................................................................... 11
HOW THIS MANUAL IS ORGANIZED ........................................................................ 11
NOTATION CONVENTIONS .......................................................................................... 11
REFLECTION LISTS ........................................................................................................ 12
CRYSTALCLEAR\d\TREK COORDINATE SYSTEM .................................................................. 13
RELATED DOCUMENTATION ....................................................................................... 14

2 INSTALLATION ............................................................................................................... 15

SYSTEM REQUIREMENTS .............................................................................................. 15
INSTALLING THE CRYPTO-BOX DONGLE .............................................................. 15
INSTALLING CRYSTALCLEAR .................................................................................. 15
AFTER INSTALLATION ................................................................................................. 16
UNINSTALLING CRYSTALCLEAR .............................................................................. 17

3 INTRODUCTION TO CRYSTALCLEAR ........................................................................... 21

WHAT IS CRYSTALCLEAR? .......................................................................................... 21
OVERVIEW OF THE CRYSTALCLEAR INTERFACE .................................................. 21
Task Drop-down List ..................................................................................................... 21
Current Sample ............................................................................................................ 21
Run Mode ..................................................................................................................... 21
Flow Bar ....................................................................................................................... 22
Step Button .................................................................................................................. 22
Steps with Substeps ..................................................................................................... 22
Toolbar ......................................................................................................................... 22

4 RUNNING CRYSTALCLEAR FOR THE FIRST TIME ...................................................... 27

STARTING CRYSTALCLEAR AND LOGGING IN .................................................. 27
CREATING YOUR FIRST PROJECT AND SAMPLE ................................................... 28
Screen Collect and Process .......................................................................................... 29
Collect and Process ..................................................................................................... 29
Collect .......................................................................................................................... 29
Process ........................................................................................................................ 29
Combine Reflections .................................................................................................... 29

5 COMMON CRYSTALCLEAR TASKS ............................................................................... 31

COLLECT IMAGES ........................................................................................................ 31
PROCESS IMAGES ........................................................................................................ 32
Setup ............................................................................................................................. 32
Assign Unit Cell .......................................................................................................... 34
Find Spots ..................................................................................................................... 34
Index Spots ................................................................................................................... 37
Table of Contents

Refine Cell .............................................................................................................................................. 38
Predict Spots ........................................................................................................................................... 40
STRATEGY ................................................................................................................................................. 41
INTEGRATE REFLECTIONS ..................................................................................................................... 42
ANALYZING THE DATA .............................................................................................................................. 43
  Laue Symmetry ....................................................................................................................................... 43
  Centricity .................................................................................................................................................. 44
  Spacegroup .............................................................................................................................................. 45
  Scale and Average ................................................................................................................................. 46

6 DATA COLLECTION AND PROCESSING ............................................................................................... 49
  SELECT A PROCESSING ALGORITHM .................................................................................................. 49
  SETUP .................................................................................................................................................... 50
  COLLECT IMAGES WITH AN IMAGING PLATE SYSTEM (R-AXIS IV) ..................................................... 57
  COLLECT IMAGES WITH CCD SYSTEM (MERCURY CCD) .................................................................. 60
  INDEX SPOTS .......................................................................................................................................... 63
    Index with d*TREK (RAXIS or CCD) .................................................................................................. 63
    Index with TwinSolve (Mercury CCD) ................................................................................................. 76
  STRATEGY ................................................................................................................................................. 80
  INTEGRATION .......................................................................................................................................... 83
    Integrate with d*TREK (RAXIS or Mercury CCD) ........................................................................... 83
  ANALYZING THE DATA ........................................................................................................................... 87
    Laue Symmetry .................................................................................................................................... 87
    Centricity .............................................................................................................................................. 87
    Spacegroup ......................................................................................................................................... 88
  SCALE AND AVERAGE ............................................................................................................................ 89
    Scale with d*TREK (RAXIS or Mercury CCD) .................................................................................. 89

7 TOOL REFERENCE .................................................................................................................................. 93
  CREATE A NEW PROJECT AND SAMPLE .............................................................................................. 93
  CREATE A NEW SAMPLE ......................................................................................................................... 94
  OPEN AN EXISTING SAMPLE ............................................................................................................... 95
  CLOSE THE CURRENT SAMPLE ......................................................................................................... 96
  SAVE THE CURRENT SAMPLE ............................................................................................................. 96
  DELETE PROJECTS AND SAMPLES ...................................................................................................... 97
  PROCESSING STATE - VIEW, EDIT AND SET ....................................................................................... 98
  CREATE A NEW PROCESSING STATE .................................................................................................. 100
  VIEW THE SCAN STATE DISPLAY ....................................................................................................... 102
    Using the Scan Table ......................................................................................................................... 103
      Manipulating the Scan Table ........................................................................................................... 105
      Editing the Scan Table ..................................................................................................................... 106
  VIEW THE INSTRUMENT STATE ........................................................................................................ 107
  MANUALLY CONTROL THE DETECTOR .............................................................................................. 108
  SET USER PREFERENCES .................................................................................................................... 110
    Configure the Instrument Server Simulator ..................................................................................... 113
      R-Axis Simulator ............................................................................................................................... 114
      CCD Simulator ................................................................................................................................. 114
  VIEW LOG FILES .................................................................................................................................. 117

8 ADDITIONAL PROCESSING ................................................................................................................... 119
  SET RESOLUTION ................................................................................................................................... 119
# Table of Contents

MEMBER REFLECTION LISTS WITH D*TREK.......................................................... 119
CREATE AND EDIT MACROS.............................................................................. 121
Creating a Macro.............................................................................................. 122
Edit a Macro..................................................................................................... 124
THE COLLECT SCHEDULE.................................................................................. 125
Create a Collect Schedule .............................................................................. 126
Import a Collect Schedule ............................................................................. 127
Save a Collect Schedule .................................................................................. 127
Run a Collect Schedule ................................................................................... 128
Delete Collection Schedule ........................................................................... 129
9 IMAGES............................................................................................................. 131
THE IMAGE WINDOW......................................................................................... 131
Large Image Window ...................................................................................... 131
Profile Windows ............................................................................................... 131
Large Image Window Toolbar ......................................................................... 132
Small Image Window Toolbar ......................................................................... 134
Small Image Window ...................................................................................... 134
Image Information Window ............................................................................ 134
APPENDIX A: FILES AND DIRECTORY STRUCTURE.......................................... 135
INSTALLED FILES.............................................................................................. 135
CrystalClear program files ............................................................................. 135
Compute Servers ............................................................................................. 135
Help Files ......................................................................................................... 135
OCX Components .......................................................................................... 136
RAXWish Files .................................................................................................. 136
Crypto-Box files .............................................................................................. 136
Additional Files .............................................................................................. 137
FILES CREATED BY CRYSTALCLEAR.............................................................. 137
DIRECTORIES..................................................................................................... 138
APPENDIX B: ADMINISTRATION....................................................................... 141
ADMINISTRATOR LOGIN.................................................................................... 141
GENERAL SETTINGS......................................................................................... 141
ADMINISTRATION OF USERS........................................................................ 142
Add a User ........................................................................................................ 143
Remove a User ............................................................................................... 144
Edit User Settings ........................................................................................... 145
ADMINISTRATION OF GROUPS....................................................................... 147
Add a Group ..................................................................................................... 147
Remove a Group ............................................................................................. 148
Edit Group Settings ......................................................................................... 148
ADMINISTRATION OF TOOLS........................................................................ 149
Add a Tool ........................................................................................................ 150
Remove a Tool ............................................................................................... 151
Edit Tool Settings ........................................................................................... 151
ADMINISTRATION OF SERVERS..................................................................... 151
Edit Server Settings......................................................................................... 152
Table of Contents

SPECIFY DEFAULT SITE-LEVEL SETTINGS.............................................................................. 154
SET UP IMAGE COLLECTION DEVICE TYPE......................................................................... 155
DETERMINE DIRECT BEAM POSITION.................................................................................. 156
CHECK PMT (PHOTOMULTIPLIER TUBE)............................................................................... 158
CONTINUOUSLY READING AN IP......................................................................................... 158

APPENDIX C: SAMPLE LOG FILES..................................................................................... 161
FIND SPOTS LOG..................................................................................................................... 162
INDEX SPOTS LOG................................................................................................................ 163
REFINE SPOTS LOG.............................................................................................................. 165
PREDICT LOG........................................................................................................................ 168
STRATEGY LOG..................................................................................................................... 170
INTEGRATE LOG.................................................................................................................... 171
LAUE LOG.............................................................................................................................. 179
CENTRICITY LOG.................................................................................................................. 180
SPACEGROUP LOG............................................................................................................... 180
SCALE AND AVERAGE LOG................................................................................................. 184
DIRECT BEAM LOG............................................................................................................... 194
PMTCHECK LOG.................................................................................................................. 196
CONTINUOUS IP READ LOG.................................................................................................. 197

APPENDIX D: TROUBLESHOOTING................................................................................... 199
GENERAL CRYSTALCLEAR PROBLEMS............................................................................. 199
CRYPTO-BOX MESSAGES...................................................................................................... 200

APPENDIX E: ABSORPTION IN SCALING............................................................................ 201

APPENDIX F: DEFAULTS IN CRYSTALCLEAR.................................................................... 205
New Sample Defaults.......................................................................................................... 205
Inherited Defaults................................................................................................................ 205
Updating Defaults.............................................................................................................. 206
Dialog Defaults.................................................................................................................... 206
Using the Default Manager.................................................................................................. 209

APPENDIX G: CRYSTALLOGRAPHIC TROUBLESHOOTING............................................... 211

INDEX.................................................................................................................................. 215
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 CrystalClear 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.
About This Manual

- 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:

<table>
<thead>
<tr>
<th>4</th>
<th>7</th>
<th>1</th>
<th>4 integers, 7 floats, 1 string</th>
</tr>
</thead>
<tbody>
<tr>
<td>nH</td>
<td>3 integer field labels</td>
<td></td>
<td></td>
</tr>
<tr>
<td>nK</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>nL</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fIntensity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fSigma</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fObs_rot_mid</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fObs_rot_width</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fResolution</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fLPfactor</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fCorrelation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>sBatch</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>-1</td>
<td>16 3566.77 121.549 … 1001</td>
<td>actual reflection file with 3 integers, 7 floats (2 shown), and one string</td>
</tr>
</tbody>
</table>
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**
About This Manual

All detector translations and rotations
All trans
X/Trans1 Detector translation along X
Y /Trans2 Detector translation along Y
Dist/Trans3 Detector translation along Z
All rots
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 R-Axis, 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:

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

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,
Installation

1. Place the CrystalClear CD in your CDROM drive.

2. Click the Start button, then click Run.

3. Enter $d:\text{setup}$, where $d$ is the drive letter of your CDROM drive, then press (Enter).

   The Welcome dialog will appear.

   ![Welcome dialog](image)

   Welcome to the CrystalClear Setup program. This program will install CrystalClear on your computer.
   
   It is strongly recommended that you exit all Windows programs before running this Setup program.
   
   Click Cancel to quit Setup and then close any programs you have running. Click Next to continue with the Setup program.
   
   WARNING: This program is protected by copyright law and international treaties.
   
   Unauthorized reproduction or distribution of this program, or any portion of it, may result in severe civil and criminal penalties, and will be prosecuted to the maximum extent possible under law.
   
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 $C:\text{PROGRAM FILES}\text{RIGAKU MSC}\text{CRYSTALCLEAR}$. 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 page 135 for information on the files that are installed, and the directory structure that is created during the installation.

After installation
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.
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.
Introduction to CrystalClear

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.
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.
Introduction to CrystalClear

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 toggled 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.
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.
Running CrystalClear for the First Time

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.
Running CrystalClear for the First Time

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.
Common CrystalClear Tasks

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.
Common CrystalClear Tasks

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
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 2θ, 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.
Right-click an entry field for further menu options as follows:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>View Images List</td>
<td>Displays a list of image files</td>
</tr>
<tr>
<td>Select Scan</td>
<td>Allows user to select images of a scan</td>
</tr>
<tr>
<td>Clear Scan</td>
<td>Clears selected images of a scan</td>
</tr>
</tbody>
</table>
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.

*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.
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**.
Common CrystalClear Tasks

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.
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 Refine** 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/σ (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/σ** 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

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 (un-highlight) the To Use entry field to verify the selected image entries.

Right-click the “To Use” field for further menu options as follows:

<table>
<thead>
<tr>
<th>Menu Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>View Images List</td>
<td>Displays a list of image files</td>
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<tr>
<td>Select Scan</td>
<td>Allows user to select images of a scan</td>
</tr>
<tr>
<td>Clear Scan</td>
<td>Clears selected images of a scan</td>
</tr>
</tbody>
</table>

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.
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**.
Common CrystalClear Tasks

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.

![Integrate Reflections Dialog](image)

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 image 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 the “To Use” field for further menu options as follows:

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</tr>
<tr>
<td>Clear Scan</td>
<td>Clears selected images of a scan</td>
</tr>
</tbody>
</table>

   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.
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 **Non-uniformity 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 completed, data may be analyzed to determine Laue symmetry, centricity, and spacegroup. See **Section 6 Data Collection and Processing** on page 49 for 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
Highest Laue Symmetry
Only check Laue groups compatible with current cell
Average Bijvoets (Assume $1+ = 1-$)

Tolerance for considering a Laue class present
Limits the highest Laue class to be checked.
Unchecked, examines all Laue classes compatible with current cell
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.
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.
Common CrystalClear Tasks

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 collected 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.
Data Collection and Processing

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 2θ, 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 (° 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 2θ (°): Swing angle of the goniometer. If you are processing existing images, the value specified when the images were collected will be displayed.
Note: Crystal To Detector Distance (mm) and Detector 2θ (°) 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.
Data Collection and Processing

Unit Cell Parameters:  The unit cell parameters for the cell.

- a (Å) default = 50.000000
- b (Å) default = 100.000000
- c (Å) 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.
Data Collection and Processing

**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/ 2θ (°)** can also be set on the **Main** 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.

**Setup**

![Setup Screen](image)

**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.
**Data Collection and Processing**

**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.
Several common schedules are:
- One: 0 (collects one image at φ = 0°)
- Two: 0,30 (collects one image at φ 0°, and one at 30°)
- Four: 0,30,60,90 (collects images at φ = 0°, 30°, 60°, and 90°)
Default Screen Schedule

**Scan Table:**
The **Scan Table** 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...
Data Collection and Processing

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:


**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.
Data Collection and Processing

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:
Data Collection and Processing

<table>
<thead>
<tr>
<th>Start Angle</th>
<th>End Angle</th>
<th>Width</th>
<th>Step</th>
<th># Images</th>
<th>Completeness</th>
<th>Start #</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>90.0</td>
<td>0.50</td>
<td>0.50</td>
<td>180</td>
<td>---</td>
<td>1</td>
</tr>
</tbody>
</table>

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.

   **Double-Check Settings**

   Please make sure that the Crystal-to-Detector Distance and Detector 2-theta Angle are correct before continuing.

   ![Double-Check Settings](image)

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*
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.
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 (un-highlight) the To Use entry field to verify the selected image entries.

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

<table>
<thead>
<tr>
<th>View Images List</th>
<th>Displays a list of image files</th>
</tr>
</thead>
<tbody>
<tr>
<td>Select Scan</td>
<td>Allows user to select images of a scan</td>
</tr>
<tr>
<td>Clear Scan</td>
<td>Clears selected images of a scan</td>
</tr>
</tbody>
</table>

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.
### Data Collection and Processing

**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.*
Data Collection and Processing

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.
Data Collection and Processing

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.

   ![Index Spots](image)

   **Max Cell Length**
   - 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.*

8. In the **Max Residual field**, specify the maximum allowed least squares residual for a solution to be
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, & Rossmann1 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.

\[ F = \sum_{i=1}^{n} \cos[2\pi (\vec{d}_i \cdot \vec{x})] \]

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 axes2.

Reciprocal Space: The reciprocal space method of Sparks is used3.


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.

---

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.
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.

### Macro Editor

<table>
<thead>
<tr>
<th>Step Name</th>
<th>Min Res</th>
<th>Max Res</th>
<th>Num Cycles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step1</td>
<td>100.0</td>
<td>3.0</td>
<td>100</td>
</tr>
</tbody>
</table>

#### Crystal
- All Crystal
- All Cell
- All Lengths
- All Angles
- All Rotations
- a
- b
- c
- α
- β
- γ
- Rot1
- Rot2
- Rot3
- Mosaicity

#### Detector
- All Detector
- All Translations
- All Rotations
- Trans1
- Trans2
- Trans3
- Rot1
- Rot2
- Rot3

#### Source
- All Rotations
- Wavelength
- Rot1
- Rot2

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 (Δλ/λ). 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.
Data Collection and Processing

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

![Overlay of above 3 images.](image)

Figure 1. 2D vs. 3D spot considerations

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 $\alpha$, $\beta$, and $\gamma$ 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
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 \( \alpha, \beta, \gamma \) 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 image 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:

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>View Images List</td>
<td>Displays a list of image files</td>
</tr>
<tr>
<td>Select Scan</td>
<td>Allows user to select images of a scan</td>
</tr>
<tr>
<td>Clear Scan</td>
<td>Clears selected images of a scan</td>
</tr>
</tbody>
</table>

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.**
Data Collection and Processing

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 Distances**.

   *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.
Data Collection and Processing

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.
Data Collection and Processing

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.
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.
2. In **Search Resolution** group box, make changes to setting by clicking **Set** button. The **Set Resolution** dialog appears:

3. Click the Advanced tab.

*For assistance in using the **Set Resolution** dialog, see page 119 in Section 8 Additional Processing.*
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 wish 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.
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.

   ![Integrate Reflections dialog](image)

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*...
Data Collection and Processing

**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:

<table>
<thead>
<tr>
<th>Menu Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>View Images List</td>
<td>Displays a list of image files</td>
</tr>
<tr>
<td>Select Scan</td>
<td>Allows user to select images of a scan</td>
</tr>
<tr>
<td>Clear Scan</td>
<td>Clears selected images of a scan</td>
</tr>
</tbody>
</table>

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 119 of 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—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 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...
Data Collection and Processing

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 $0.5 \times \arctan\left(\frac{\text{spot_size}}{\text{crystal_to_detector_distance}}\right)$ and $\max(\text{crystal_mosaicity}/3, 2 \times \text{image_rotation_width})$. 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.
Data Collection and Processing

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.
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:

<table>
<thead>
<tr>
<th>Setting</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max R-merge</td>
<td>Tolerance for considering a Laue class present</td>
</tr>
<tr>
<td>Highest Laue Symmetry</td>
<td>Limits the highest Laue class to be checked.</td>
</tr>
<tr>
<td>Only check Laue groups compatible with current cell</td>
<td>Unchecked, examines all Laue classes compatible with current cell</td>
</tr>
<tr>
<td>Average Bijvoets (Assume 1+ = 1-)</td>
<td>Unchecked examines Laue classes desired</td>
</tr>
</tbody>
</table>

4. Click Run.

Centricity

Data Collection and Processing

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
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. **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.
Data Collection and Processing

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 $f\sigma_I$ values set to 0 or less.
Data Collection and Processing

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 (sigmal <= 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 Projects 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.
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).**
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.
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,

   ![Close Sample Dialog]

   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.
• Alternatively, access the save feature from the CrystalClear 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.

   ![CrystalClear dialog](image1)

   The following CrystalClear dialog appears. To continue with the delete procedure, read the warning and click OK.

   ![CrystalClear dialog](image2)

   The Delete Projects/Samples dialog will appear.
2. Select (highlight) the project or sample you wish to delete, then click the appropriate **Delete Project(s)** or **Delete 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**.
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
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.
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

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.
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

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 **CrystalClear** 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**:

<table>
<thead>
<tr>
<th>Scan ID</th>
<th>Template</th>
<th>Dist</th>
<th>2θ</th>
<th>sin Christianity</th>
<th>Angle</th>
<th>Angle</th>
<th>Wavelength</th>
<th># Complete</th>
<th>Start</th>
<th>Exp</th>
<th>Total</th>
<th>Collected</th>
<th>Schedule</th>
<th>Start</th>
<th>End</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>Nylo2000.png</td>
<td>28.0</td>
<td>0.0</td>
<td>53.4</td>
<td>45.0</td>
<td>90.0</td>
<td>30.0</td>
<td>30.0</td>
<td>0.50</td>
<td>120</td>
<td>361</td>
<td>4.0</td>
<td>301-600</td>
<td>301-600</td>
<td>35.0</td>
</tr>
<tr>
<td>19</td>
<td>Nylo2000.png</td>
<td>20.0</td>
<td>0.0</td>
<td>53.4</td>
<td>45.0</td>
<td>90.0</td>
<td>30.0</td>
<td>30.0</td>
<td>0.50</td>
<td>120</td>
<td>401</td>
<td>5.0</td>
<td>481-600</td>
<td>481-600</td>
<td>35.0</td>
</tr>
</tbody>
</table>

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-θ* (*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**

**Phi** ($\phi$): Specify the position of the crystal goniometer in degrees.

**Rotation Axis:** Phi ($\phi$). (Phi ($\phi$) 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:** The **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 Columns 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.
Right-click column entries: Depending upon the particular column entry, a useful pop-up 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.*
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:

<table>
<thead>
<tr>
<th>Start Angle</th>
<th>End Angle</th>
<th>Width</th>
<th>Step</th>
<th># Images</th>
<th>Completeness</th>
<th>Start #</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>90.0</td>
<td>0.50</td>
<td>0.50</td>
<td>180</td>
<td>---</td>
<td>1</td>
</tr>
</tbody>
</table>

**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 appear.
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
• 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.
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.
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.
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**
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.

![Image of Preferences dialog]

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.
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*.

\[
\text{SimulatorBaseFilename} = \text{drive:}\backslash\text{path}\backslash\text{base}
\]

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:*
\(\backslash\text{path}\backslash\text{base}\ ???\).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).

\[
\text{SimulatorMode} = \text{realtime} | \text{immediate}
\]

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).

\[
\text{SimulatorBaseFilename} = \text{drive:}\backslash\text{path}\backslash\text{base}
\]

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:*
\(\backslash\text{path}\backslash\text{base}\ ???\).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. 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.

\textit{SimulatorMode = realtime | immediate}

This option indicates if the simulator will mimic real time when simulating exposures. If the value is \textit{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 \textit{immediate}, then the exposures will finish immediately.

**Specify User Preferences**

To customize other user preferences,

1. Click \textbf{Tools > Preferences} on the menu. The \textit{Preferences} dialog will appear.

2. Click the \textit{General} tab.
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.
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.
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.

![Set Resolution Dialog]

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.
Additional Processing

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 ReflectionLists 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,
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 **Filename** 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.

![Select Reflection File to Import](image)

**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
Additional Processing

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.*

![Macro Editor dialog](Image)
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.
Additional Processing

**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.
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 Collect.)
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.
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.
Additional Processing

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

![Default Manager dialog](image)

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)
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.
Additional Processing

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.

![Image of Scan State Display window]

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**.
9 Images

The Image Window

*CrystalClear* offers a graphical view of your data in the 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.

**Large Image Window**

The profile windows display a graphical profile, showing you the values of the pixels that intersect the x- and 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.)*
Images

- **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 page 54 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.
Images

- **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 $\phi$. 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

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**

<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CrystalClear.exe</td>
<td>Executable program file</td>
</tr>
<tr>
<td>CoreCode11.dll</td>
<td>Shared code program library</td>
</tr>
<tr>
<td>CoreRes11ENG.dll</td>
<td>English language resource file</td>
</tr>
<tr>
<td>CoreHobject11.dll</td>
<td>DLL for database functions</td>
</tr>
<tr>
<td>gzip.exe</td>
<td>Decompression utility used to decompress image files</td>
</tr>
<tr>
<td>DundasUG.dll</td>
<td>DLL for table controls</td>
</tr>
<tr>
<td>system.configuration</td>
<td>System configuration file</td>
</tr>
<tr>
<td>xg_dll.dll</td>
<td>DLL for x-ray generator control</td>
</tr>
</tbody>
</table>

**Compute Servers**

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

**Help Files**

<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CrystalClear.chm</td>
<td>Online help file for <em>CrystalClear</em></td>
</tr>
<tr>
<td>CrystalClearDoc.pdf</td>
<td>Online Manual for <em>CrystalClear</em></td>
</tr>
<tr>
<td>CoreHelp.chm</td>
<td>Online help file for <em>CrystalClear</em></td>
</tr>
<tr>
<td>TwinSolve.chm</td>
<td>Online help file for TwinSolve module</td>
</tr>
<tr>
<td>infolist.txt</td>
<td>Readme file containing release notes and other info</td>
</tr>
<tr>
<td>hh.exe</td>
<td>HTML help engine</td>
</tr>
<tr>
<td>hhctrl.ocx</td>
<td>Help engine file</td>
</tr>
<tr>
<td>itircl.dll</td>
<td>Help engine file</td>
</tr>
</tbody>
</table>

*CrystalClear User Manual*  
Page 135
Appendix A: Files and Directory Structure Images

**OCX Components**

- itss.dll: Help engine file
- popup.ocx: Help engine file
- 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**

<table>
<thead>
<tr>
<th>File</th>
<th>Compatibility</th>
</tr>
</thead>
<tbody>
<tr>
<td>Version.txt</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Cbn.vxd</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Install.bat</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Marx.reg</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Readme.txt</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Cbn.inf</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Register.bat</td>
<td>(Win95/98)</td>
</tr>
<tr>
<td>Marxdev1.ini</td>
<td>(WinNT)</td>
</tr>
<tr>
<td>Marxdev1.reg</td>
<td>(WinNT)</td>
</tr>
<tr>
<td>Marxdev1.sys</td>
<td>(WinNT)</td>
</tr>
<tr>
<td>Marxdev2.ini</td>
<td>(WinNT)</td>
</tr>
<tr>
<td>Marxdev2.reg</td>
<td>(WinNT)</td>
</tr>
<tr>
<td>Marxdev2.sys</td>
<td>(WinNT)</td>
</tr>
<tr>
<td>Marxdev3.ini</td>
<td>(WinNT)</td>
</tr>
</tbody>
</table>
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.
Appendix A: Files and Directory Structure Images

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

**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.
Appendix B: Administration

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 account has no password (blank). A new password for the Administrator account should be set by using the procedure to Edit User Settings on page 145 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.
Appendix B: Administration

To set defaults, access the Administration dialog.
1. At the menu line, click Tools > Administration.
   The Administration dialog will appear.

![Administration Dialog Image]

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*
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.
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.*
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.

![CrystalClear dialog]

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.
Appendix B: Administration

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.
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.
Appendix B: Administration

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.
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.
Appendix B: Administration

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.
Appendix B: Administration

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.

![Administration Dialog]

**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.
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.
Appendix B: Administration

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.
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 project as it is created. Users can modify these settings 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.
Appendix B: Administration


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.

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
In order to correctly process data that have been collected on the instrument, the position of the direct X-ray 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.


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.
Appendix B: Administration

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 X on the upper-right of the dialog box.

Check PMT (PhotoMultipler 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 X 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 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 R-AXIS 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 Utilities 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**

<table>
<thead>
<tr>
<th>Process</th>
<th>Log Filename</th>
</tr>
</thead>
<tbody>
<tr>
<td>Find Spots</td>
<td>dtfind.log</td>
</tr>
<tr>
<td>Refine Spots</td>
<td>drefine.log</td>
</tr>
<tr>
<td>Index Spots</td>
<td>dtindex.log</td>
</tr>
<tr>
<td>Predict Spots</td>
<td>dtpredictspots.log</td>
</tr>
<tr>
<td>Integrate Spots</td>
<td>dtintegrate.log</td>
</tr>
<tr>
<td>Scale and Merge</td>
<td>dtscalemerge.log</td>
</tr>
<tr>
<td>Merge Reflections</td>
<td>dtreflectionmerge.log</td>
</tr>
<tr>
<td>Strategy</td>
<td>dtstrategy.log</td>
</tr>
</tbody>
</table>

For **PROCESS**

<table>
<thead>
<tr>
<th>Process</th>
<th>Log Filename</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak Search</td>
<td>psearch.log</td>
</tr>
<tr>
<td>Index</td>
<td>index.log</td>
</tr>
<tr>
<td>Refine</td>
<td>refosc.log</td>
</tr>
<tr>
<td>Integrate</td>
<td>integ.log</td>
</tr>
<tr>
<td>Merge</td>
<td>merge.log</td>
</tr>
<tr>
<td>Scale</td>
<td>scale.log</td>
</tr>
<tr>
<td>Post Refine</td>
<td>post.log</td>
</tr>
<tr>
<td>Average</td>
<td>average.log</td>
</tr>
</tbody>
</table>

For **TwinSolve**

<table>
<thead>
<tr>
<th>Process</th>
<th>Log Filename</th>
</tr>
</thead>
</table>

The log files are stored in the Sample directory.
Appendix C: Sample Log Files

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.
```
Appendix C: Sample Log Files

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:

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
14Verbose:  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
Appendix C: Sample Log Files

sorted on decreasing (highest to lowest) symmetry.
Only solutions with residuals <= 10.0 are listed.

<table>
<thead>
<tr>
<th>Soln</th>
<th>LeastSq</th>
<th>Spgrp</th>
<th>Cent</th>
<th>Bravais</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>type</th>
<th>alpha</th>
<th>beta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.789</td>
<td>P</td>
<td>75</td>
<td>tetragonal</td>
<td>71.698</td>
<td>71.698</td>
<td>106.730</td>
<td>90.000 90.000 90.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>3.735</td>
<td>C</td>
<td>21</td>
<td>orthorhombic</td>
<td>100.969</td>
<td>101.820</td>
<td>106.730</td>
<td>90.000 90.000 90.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>3.677</td>
<td>C</td>
<td>5</td>
<td>monoclinic</td>
<td>100.969</td>
<td>101.820</td>
<td>106.730</td>
<td>90.000 90.335 90.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1.130</td>
<td>P</td>
<td>16</td>
<td>orthorhombic</td>
<td>69.244</td>
<td>74.070</td>
<td>106.730</td>
<td>90.000 90.000 90.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.638</td>
<td>P</td>
<td>3</td>
<td>monoclinic</td>
<td>74.070</td>
<td>69.244</td>
<td>106.730</td>
<td>90.000 90.457 90.000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.000</td>
<td>P</td>
<td>1</td>
<td>triclinic</td>
<td>69.244</td>
<td>74.070</td>
<td>106.730</td>
<td>90.457 90.000 90.482</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Suggested spacegroup number until systematic absences are examined.
Enter solution number of your choice: 10
Solution number 10 selected.

Unit cell parameters and orientation angles

<table>
<thead>
<tr>
<th>Integer</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>Rot1</th>
<th>Rot2</th>
<th>Rot3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>69.241</td>
<td>74.081</td>
<td>106.637</td>
<td>155.782</td>
<td>30.261</td>
<td>102.479</td>
</tr>
<tr>
<td></td>
<td>89.463</td>
<td>90.013</td>
<td>89.579</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>69.241</td>
<td>74.081</td>
<td>106.637</td>
<td>-155.782</td>
<td>-30.261</td>
<td>-77.521</td>
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<tr>
<td></td>
<td>90.537</td>
<td>89.987</td>
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<td></td>
<td></td>
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</tr>
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<td>69.241</td>
<td>74.081</td>
<td>106.637</td>
<td>24.218</td>
<td>-30.261</td>
<td>-77.521</td>
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<td>90.537</td>
<td>90.013</td>
<td>90.421</td>
<td></td>
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</tr>
<tr>
<td>4</td>
<td>69.241</td>
<td>74.081</td>
<td>106.637</td>
<td>-24.218</td>
<td>30.261</td>
<td>102.479</td>
</tr>
<tr>
<td></td>
<td>89.463</td>
<td>89.987</td>
<td>90.421</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Enter your choice: 1
Orientation angles choice 1 selected.

Crystal listing:

Unit cell lengths: 69.2409 74.0809 106.6370
Unit cell angles: 90.0000 90.0000 90.0000
Unit cell volume: 546986.750
Orientation angles: 155.7821 30.2615 102.4790
Mosaicity: 0.300
Description: unknown

Spacegroup number: 16
name: P222
Num. equiv. posns: 4
dtindex - Wrote header file dtindex.head
DTREK_STATUS: 0
Appendix C: Sample Log Files

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:
Appendix C: Sample Log Files

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
18 Name          Datum   Current  Units   Vector
19 ==============================================================
20 Omega         0.000   Unknown   deg   ( 1.000, 0.000, 0.000)
21 Chi           0.000   Unknown   deg   ( 0.000, 1.000, 0.000)
22 Phi           0.000   Unknown   deg   ( 1.000, 0.000, 0.000)
23 ==============================================================
24 Source listing:
25 Single wavelength: 1.5418
26 Polarization: 0.5, 1, 0, 0
27 Intensity: 0
28 RX_Detector listing:
29 Pixel dimensions: 1900, 1900
30 Nominal size in mm: 193.23, 199.5
31 Description: RAXIS conversion
32 RX_Goniometer listing:
33 Description: UNKNOWN
34 Number of values: 6
35
36 Name              Datum   Current  Units   Vector
37 ==============================================================
38 RotZ              0.000   Unknown   deg   ( 0.000, 0.000, 1.000)
39 RotX/Swing        0.000   Unknown   deg   (-1.000, 0.000, 0.000)
40 RotY              0.000   Unknown   deg   ( 0.000, 1.000, 0.000)
41 TransX            0.000   Unknown   mm    ( 1.000, 0.000, 0.000)
42 TransY            0.000   Unknown   mm    ( 0.000, 1.000, 0.000)
43 TransZ/Dist       98.000   Unknown   mm    ( 0.000, 0.000, -1.000)
44 ==============================================================
45 DetResolution min: 154180
46 DetResolution max: 1.6678
47 Refine resol min: 99999
48 Refine resol max: 1e-05
49 I/sigma cutoff: 0
50 Rejection limits: 1, 1, 2
51 Rel. rot. weight: 9999
52 Refinement results
53 ==============================================================
54 Crystal
55 a, b, c: 68.6284 73.7186 106.5789
56 Sigmas: 0.0170 0.0102 0.0235
57 Shifts: 0.0000 0.0000 0.0000
Appendix C: Sample Log Files

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.
Appendix C: Sample Log Files

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

dtpredict: Copyright (c) 1996 Molecular Structure Corporation
1 d*TREK version 6.1SSI -- Oct 27 2000
2 Command line:
3   dtpredict input.head -seq 180 180 -mosaicity 0.60 -out output.head -ref \\n4       dtpredict.ref -display -list
5     Header of file input.head successfully read.
6
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
16 Predict listing:

17   Spacegroup number: 96
18      name: P43212
19   Num. equiv. posns: 8
20  Equival. position 1:
21    1, 0, 0    0
22    0, 1, 0    0
23    0, 0, 1    0
24  Equival. position 2:
25    -1, 0, 0    0
26    0, -1, 0    0
27    0, 0, 1    0.5
28  Equival. position 3:
29    0, 1, 0    0 0.5
30    -1, 0, 0    0 0.5
31    0, 0, 1    0.75
32  Equival. position 4:
33    0, -1, 0    0 0.5
34    1, 0, 0    0 0.5
35    0, 0, 1    0.25
36  Equival. position 5:
37    0, 1, 0    0
38    1, 0, 0    0
39    0, 0, -1   0
40  Equival. position 6:
41    0, -1, 0    0
42    -1, 0, 0    0
43    0, 0, -1   0.5
44  Equival. position 7:
45    -1, 0, 0    0 0.5
46    0, 1, 0    0 0.5
47    0, 0, -1   0.75
Appendix C: Sample Log Files

Equival. position 8:
1, 0, 0 0.5
0, -1, 0 0.5
0, 0, -1 0.25

Crystal Orientation Matrix is:

\[
\begin{bmatrix}
0 \times & -3.78606e-005 & -0.00727938 & 0.0103656 \\
[1] \times & 0.00666557 & 0.00880277 & 0.00620622 \\
[2] \times & -0.0230547 & 0.0117159 & 0.00814348
\end{bmatrix}
\]

Crystal Orientation Matrix is:

CRYSTAL_ Goniometer listing:

Description: Eulerian 3-circle
Number of values: 3

<table>
<thead>
<tr>
<th>Name</th>
<th>Datum</th>
<th>Current</th>
<th>Units</th>
<th>Vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>VirtualOmega</td>
<td>0.000</td>
<td>Unknown</td>
<td>deg</td>
<td>1.000, 0.000, 0.000</td>
</tr>
<tr>
<td>VirtualChi</td>
<td>0.000</td>
<td>Unknown</td>
<td>deg</td>
<td>0.000, 0.000, 1.000</td>
</tr>
<tr>
<td>Phi</td>
<td>0.000</td>
<td>Unknown</td>
<td>deg</td>
<td>1.000, 0.000, 0.000</td>
</tr>
</tbody>
</table>

Source listing:

Single wavelength: 1.5418
Direction vector: 0, 0, 1
Spectral Dispersion: 0.0002, 0.0002
Crossfire: 0.0002, 0.0002, 0, 0
Polarization: 0.5, 1, 0, 0
Size: 0, 0, 0, 0
Intensity: 0

RX_Detector listing:

Pixel dimensions: 3000, 3000
Nominal size in mm: 300, 300
Description: RAXIS conversion
Fast pixel vector: 1, 0, 0
Slow pixel vector: 0, 1, 0
Spatial distortion descriptive text:
Simple pixel scaling spatial distortion
Simple spatial distortion:
Center of primary beam: 1479, 1529
Pixel size (mm): 0.1, 0.1
Direction vectors: 0, 1, -1, 0

RX_ Goniometer listing:

Description: UNKNOWN
Number of values: 6

<table>
<thead>
<tr>
<th>Name</th>
<th>Datum</th>
<th>Current</th>
<th>Units</th>
<th>Vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>RotAboutBeam</td>
<td>0.169</td>
<td>Unknown</td>
<td>deg</td>
<td>0.000, 0.000, 1.000</td>
</tr>
<tr>
<td>2Theta</td>
<td>0.079</td>
<td>Unknown</td>
<td>deg</td>
<td>-1.000, 0.000, 0.000</td>
</tr>
<tr>
<td>RotY</td>
<td>0.214</td>
<td>Unknown</td>
<td>deg</td>
<td>0.000, 1.000, 0.000</td>
</tr>
<tr>
<td>XShift</td>
<td>-0.054</td>
<td>Unknown</td>
<td>mm</td>
<td>1.000, 0.000, 0.000</td>
</tr>
<tr>
<td>YShift</td>
<td>0.120</td>
<td>Unknown</td>
<td>mm</td>
<td>0.000, 1.000, 0.000</td>
</tr>
<tr>
<td>Distance</td>
<td>119.478</td>
<td>Unknown</td>
<td>mm</td>
<td>0.000, 0.000, -1.000</td>
</tr>
</tbody>
</table>

DetResolution min: 154180
DetResolution max: 1.51956
DetResolution edge: 1.76436

Rotation list:
Start: 184.500
Appendix C: Sample Log Files

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 range range shell cumul
------------------------------------
33 42.0 - 47.0 5.0 15.1 15.1

Page 170  CrystalClear User Manual
Appendix C: Sample Log Files

<table>
<thead>
<tr>
<th>Resolution range</th>
<th>Calc unique</th>
<th>Num reflns</th>
<th>Num rejs</th>
<th>Num mults</th>
<th>single unique</th>
<th>mult shell</th>
<th>Avg Calc</th>
<th>%Comp</th>
<th>%Comp cumul</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.66 - 3.78</td>
<td>2777</td>
<td>5666</td>
<td>0</td>
<td>2037</td>
<td>592</td>
<td>2629</td>
<td>2.38</td>
<td>94.7</td>
<td>94.7</td>
</tr>
<tr>
<td>3.78 - 3.01</td>
<td>2592</td>
<td>5555</td>
<td>0</td>
<td>1888</td>
<td>703</td>
<td>2591</td>
<td>2.42</td>
<td>100.0</td>
<td>97.2</td>
</tr>
<tr>
<td>3.01 - 2.63</td>
<td>2370</td>
<td>5370</td>
<td>0</td>
<td>1925</td>
<td>444</td>
<td>2369</td>
<td>2.45</td>
<td>100.0</td>
<td>98.1</td>
</tr>
<tr>
<td>2.63 - 2.39</td>
<td>2370</td>
<td>5333</td>
<td>0</td>
<td>1814</td>
<td>666</td>
<td>2480</td>
<td>2.40</td>
<td>100.0</td>
<td>98.5</td>
</tr>
<tr>
<td>2.39 - 2.22</td>
<td>2370</td>
<td>5333</td>
<td>0</td>
<td>1814</td>
<td>555</td>
<td>2369</td>
<td>2.49</td>
<td>100.0</td>
<td>98.8</td>
</tr>
<tr>
<td>2.22 - 2.09</td>
<td>2666</td>
<td>6185</td>
<td>0</td>
<td>2222</td>
<td>444</td>
<td>2666</td>
<td>2.49</td>
<td>100.0</td>
<td>99.0</td>
</tr>
<tr>
<td>2.09 - 1.98</td>
<td>2370</td>
<td>5148</td>
<td>0</td>
<td>1814</td>
<td>555</td>
<td>2369</td>
<td>2.41</td>
<td>100.0</td>
<td>99.1</td>
</tr>
<tr>
<td>1.98 - 1.89</td>
<td>2481</td>
<td>5259</td>
<td>0</td>
<td>1888</td>
<td>592</td>
<td>2480</td>
<td>2.36</td>
<td>100.0</td>
<td>99.2</td>
</tr>
<tr>
<td>1.89 - 1.82</td>
<td>2185</td>
<td>5037</td>
<td>0</td>
<td>1666</td>
<td>518</td>
<td>2184</td>
<td>2.54</td>
<td>100.0</td>
<td>99.3</td>
</tr>
<tr>
<td>1.82 - 1.76</td>
<td>2629</td>
<td>5259</td>
<td>0</td>
<td>1777</td>
<td>777</td>
<td>2554</td>
<td>2.36</td>
<td>97.1</td>
<td>99.1</td>
</tr>
</tbody>
</table>

23.66 - 1.76  24921  54108  0  18845  5846  24691  2.43  99.1  99.1

*** 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:

```
integrate: Copyright (c) 1996 Molecular Structure Corporation
Header of file dtrefine.head successfully read.
RX_NONUNF_TYPE: >>None<<

Command line string: >>-reso<<
Command line string: >>-window<<
Command line string: >>-pad<<
Command line string: >>-profsize<<
Command line string: >>-batch<<
Command line string: >>-display<<
Command line string: >>-seq<<

Integrate object listing:

<table>
<thead>
<tr>
<th>Verbos level:</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scan sequence range:</td>
<td>1, 20</td>
</tr>
<tr>
<td>Resolution range:</td>
<td>100, 3</td>
</tr>
<tr>
<td>Images/batch:</td>
<td>5</td>
</tr>
<tr>
<td>Batch prefix:</td>
<td></td>
</tr>
<tr>
<td>Image padding:</td>
<td>2</td>
</tr>
<tr>
<td>Window size:</td>
<td>30, 30</td>
</tr>
<tr>
<td>Profile size:</td>
<td>0.5, 0.5</td>
</tr>
</tbody>
</table>
```

CrystalClear User Manual  Page 171
dtintegrate: 3D method used
RX_NONUNF_TYPE: >>None<<

File /user4//DATA/NUCL4/nucl4001.osc successfully opened.

IMAGE #: 1  (of 20)
Name: /user4//DATA/NUCL4/nucl4001.osc
Date: 25-Sep-1997
Time: 14:53:12

Rotation list:
Start:   24.000
End:   24.250
Increment:    0.250
Time:  120.000

Reflection dispositions
Status:    New  Active    Full   DNormal DSpecial
Number:    340     340       0       0       0

Shoebox dispositions
Status:  Total Filling    Full   Freed
Number:   1951     340       0    1611

Refinement options found:
+CrysAll +DetAll -rej 1.0 1.0 2.0 -cycles 10 -weight 9999 -display -go

File /user4//DATA/NUCL4/nucl4020.osc successfully opened.

IMAGE #: 20  (of 20)
Name: /user4//DATA/NUCL4/nucl4020.osc
Date: 25-Sep-1997
Time: 14:58:28

Rotation list:
Start:   28.750
End:   29.000
Increment:    0.250
Time:  120.000

Reflection dispositions
Status:    New  Active    Full   DNormal DSpecial
Number:      0     338     338     648      90

Shoebox dispositions
Status:  Total Filling    Full   Freed
Number:   1951       0     738    1213
Appendix C: Sample Log Files

<table>
<thead>
<tr>
<th>Unit cell lengths: 68.7533 73.7744 107.0866</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unit cell angles: 90.0000 90.0000 90.0000</td>
</tr>
<tr>
<td>Orientation angles: 155.9357 29.9512 102.4337</td>
</tr>
<tr>
<td>Mosaicity: 0.480</td>
</tr>
<tr>
<td>Description: unknown</td>
</tr>
<tr>
<td>Spacegroup number: 16</td>
</tr>
<tr>
<td>name: P222</td>
</tr>
<tr>
<td>Num. equiv. posns: 4</td>
</tr>
<tr>
<td>CRYS_TAL_Goniometer listing:</td>
</tr>
<tr>
<td>Description: Eulerian 3-circle</td>
</tr>
<tr>
<td>Number of values: 3</td>
</tr>
<tr>
<td>Name</td>
</tr>
<tr>
<td>-------------</td>
</tr>
<tr>
<td>Omega</td>
</tr>
<tr>
<td>Chi</td>
</tr>
<tr>
<td>Phi</td>
</tr>
<tr>
<td>Source listing:</td>
</tr>
<tr>
<td>Single wavelength: 1.5418</td>
</tr>
<tr>
<td>Polarization: 0.5, 1, 0, 0</td>
</tr>
<tr>
<td>Intensity: 0</td>
</tr>
<tr>
<td>RX_Detector listing:</td>
</tr>
<tr>
<td>Pixel dimensions: 1900, 1900</td>
</tr>
<tr>
<td>Nominal size in mm: 193.23, 199.5</td>
</tr>
<tr>
<td>Description: RAXIS conversion</td>
</tr>
<tr>
<td>RX_Goniometer listing:</td>
</tr>
<tr>
<td>Description: UNKNOWN</td>
</tr>
<tr>
<td>Number of values: 6</td>
</tr>
<tr>
<td>Name</td>
</tr>
<tr>
<td>-------------</td>
</tr>
<tr>
<td>RotZ</td>
</tr>
<tr>
<td>RotX/Swing</td>
</tr>
<tr>
<td>RotY</td>
</tr>
<tr>
<td>TransX</td>
</tr>
<tr>
<td>TransY</td>
</tr>
<tr>
<td>TransZ/Dist</td>
</tr>
<tr>
<td>DetResolution min: 154180</td>
</tr>
<tr>
<td>DetResolution max: 1.66982</td>
</tr>
<tr>
<td>Refine resol min: 99999</td>
</tr>
<tr>
<td>Refine resol max: 1e-05</td>
</tr>
<tr>
<td>I/sigma cutoff: 0</td>
</tr>
<tr>
<td>Rejection limits: 1, 1, 2</td>
</tr>
<tr>
<td>Rel. rot. weight: 9999</td>
</tr>
<tr>
<td>Refinement results</td>
</tr>
<tr>
<td>Crystal</td>
</tr>
<tr>
<td>a, b, c: 68.7510 73.7993 107.0777</td>
</tr>
<tr>
<td>Sigmas: 0.0032 0.0025 0.0053</td>
</tr>
<tr>
<td>Shifts: 0.0000 0.0000 0.0000</td>
</tr>
</tbody>
</table>
## Appendix C: Sample Log Files

| 157 | alpha, beta, gamma: | 90.0000 | 90.0000 | 90.0000 |
| 158 | Sigmas:            | fixed   | fixed   | fixed   |
| 159 | Shifts:           | fixed   | fixed   | fixed   |
| 160 | Crys Rot1, Rot2, Rot3: | 155.938 | 29.965 | 102.437 |
| 161 | Sigmas:           | 0.0012  | 0.0011  | 0.0035  |
| 162 | Shifts:           | 0.0000  | 0.0000  | 0.0000  |
| 163 | Mosaicity:        | 0.442   |         |         |
| 164 | Sigma:            | 0.0221  |         |         |
| 165 | Shift:            | 0.0000  |         |         |
| 166 | Detector:         | 0       |         |         |
| 167 | Trans1, Trans2, Trans3: | 0.095   | 0.058  | 98.009  |
| 168 | Sigmas:           | 0.0185  | 0.0138  | 0.0358  |
| 169 | Shifts:           | 0.0000  | 0.0000  | 0.0000  |
| 170 | Det Rot1, Rot2, Rot3: | 0.252   | -0.024 | -0.043  |
| 171 | Sigmas:           | 0.0166  | 0.0082  | 0.0085  |
| 172 | Shifts:           | 0.0002  | 0.0000  | 0.0000  |
| 173 | Source            |         |         |         |
| 174 | Wavelength, Rot1, Rot2: | 1.5418  | 0.000  | 0.000   |
| 175 | Sigmas:           | fixed   | fixed   | fixed   |
| 176 | Shifts:           | fixed   | fixed   | fixed   |
| 177 | Refinement residuals |
| 178 | rmsResid (mm)    | 0.0724333 |
| 179 | rmsResid (Deg)   | 0.0393826 |
| 180 | Reflections in list: 648 |
| 181 | Reflections accepted: 645 |
| 182 | Reflections rejected: 3 |
| 183 | Reflections ignored: 0 (Outside I/sigI or Resolution limits) |
| 184 | Strong peak info listing |

| 185 | Area | Num | Intensity | Sigma | BackAvg | BackSig | Siz0 | Siz1 | Siz2 | Dl | Shft0 | Shft1 | Shft2 |
| 186 | 1    | 0   | 0        | 0     | 0       | 0       | 0.0  | 0.0  | 0.0  | 0  | 0.0   | 0.0   | 0.0   |
| 187 | 2    | 8   | 824481   | 1482  | 705     | 0.0     | 84   | 13.0 | 12.6 | 3.0| -0.9  | 0.1   | 0.0   |
| 188 | 3    | 22  | 1667487  | 2064  | 831     | 0.0     | 92   | 12.7 | 14.5 | 4.8| 0.1   | 0.0   | 0.0   |
| 189 | 4    | 21  | 1296592  | 1936  | 854     | 0.0     | 89   | 13.2 | 13.5 | 5.9| -0.5  | 0.3   | 0.0   |
| 190 | 5    | 15  | 578864   | 1376  | 774     | 0.0     | 84   | 12.9 | 11.8 | 3.1| 0.0   | 0.6   | 0.0   |
| 191 | 6    | 0   | 0        | 0     | 0       | 0       | 0.0  | 0.0  | 0.0  | 0  | 0.0   | 0.0   | 0.0   |
| 192 | 7    | 0   | 0        | 0     | 0       | 0       | 0.0  | 0.0  | 0.0  | 0  | 0.0   | 0.0   | 0.0   |
| 193 | 8    | 133 | 783169   | 1433  | 820     | 0.0     | 88   | 14.4 | 10.2 | 2.8| -0.5  | 0.5   | 0.0   |
| 194 | 9    | 116 | 871217   | 1401  | 693     | 0.0     | 79   | 13.3 | 10.8 | 3.3| 0.7   | 0.0   | 0.0   |
| 195 | 10   | 101 | 802518   | 1323  | 715     | 0.0     | 74   | 13.3 | 10.7 | 3.5| -0.3  | -0.3  | 0.0   |
| 196 | 11   | 150 | 664956   | 1398  | 842     | 0.0     | 87   | 14.8 | 10.2 | 2.9| 0.1   | 0.0   | 0.0   |
| 197 | 12   | 0   | 0        | 0     | 0       | 0       | 0.0  | 0.0  | 0.0  | 0  | 0.0   | 0.0   | 0.0   |
| 198 | 13   | 0   | 0        | 0     | 0       | 0       | 0.0  | 0.0  | 0.0  | 0  | 0.0   | 0.0   | 0.0   |
| 199 | 14   | 6   | 1027184  | 1709  | 698     | 0.0     | 83   | 13.0 | 13.2 | 3.8| 0.1   | 0.9   | 0.0   |
| 200 | 15   | 22  | 961800   | 1779  | 767     | 0.0     | 89   | 12.1 | 13.4 | 4.5| 0.9   | 0.5   | 0.0   |
| 201 | 16   | 22  | 908059   | 1754  | 806     | 0.0     | 85   | 12.3 | 13.1 | 5.5| 0.0   | -0.2  | 0.0   |
| 202 | 17   | 11  | 655907   | 1430  | 714     | 0.0     | 78   | 12.6 | 12.3 | 3.9| 0.5   | -0.2  | 0.0   |
| 203 | 18   | 0   | 0        | 0     | 0       | 0       | 0.0  | 0.0  | 0.0  | 0  | 0.0   | 0.0   | 0.0   |
| 204 | All  | 627 | 828911   | 1465  | 778     | 0.0     | 84   | 13.8 | 11.0 | 3.4| 0.0   | 0.1   | 0.0   |
| 205 | Normal: 648, Special: 90, Reclassified as partial: 1 |
| 206 | Integrate: ...done. |
Appendix C: Sample Log Files

---

*** dtintegrate ***

Summary of results for scan rotation from 24.000 to 29.000 with image sequence numbers from 1 to 20

---

Total reflections predicted: 2714
Total reflections with no errors: 1687
Total reflections with bad errors*: 64
Total reflections partial in scan*: 886
Total reflections unprocessed at end: 0
Total reflection profiles written: 1764

Reflection integration status codes

<table>
<thead>
<tr>
<th>Status</th>
<th>Num reflns</th>
</tr>
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</table>

---

*Rejected from output.

dtintegrate: There were 1764 profiles written to file reflnprofiles.profit.
dtnprofit: Copyright (c) 1996 Molecular Structure Corporation
dtnprofit settings:
Minimum required contributors to a reference profile: 50
Minimum reference profile value in peak area: 0
Variance weighted profile analysis method B used.
Maximum number of reference profiles: 72
Number of reflection profiles read in: 1764
Profile Reflns Sum(Pi**2/Vi) Contributors
---

0 149 670 0 0/0 18/0 1/1 6/0 19/6 24/0 7/21 25/121
1 149 670 1 1/1 19/6 7/21 2/0 6/0 0/0 25/121
...
71 193 648 71 71/0 53/0 70/12 65/0 52/8 47/0 64/173
72 1764 620 Overall profile

File D0001.refprof successfully opened.
Success writing file D0001.refprof!
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
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 ______________________________________
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.
Appendix C: Sample Log Files

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.
Appendix C: Sample Log Files

Lines 269-270 The dtprofit module is started in order to fit profiles. This performs three-dimensional profile analysis with a method similar to that of Kabsch (1988).

Reference profiles.

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).
Appendix C: Sample Log Files

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 -anom -maxmerge 0.150000 -spacegroup 16 -laueonly
6  Header "input.head" opened.
7  Output Header Name set to "output.head".
8  Command line string: >> -head<<
9  Command line string: >> -tols<<
10 Cell tolerances set to [ 1000000.00 1000000.00 1000000.00 1000000.00 \
11 1000000.00 1000000.00]
12 Command line string: >> -anom<<
13 Laue check assumes I+ != I-
14 Command line string: >> -maxmerge<<
15 Maximum R-merge is 0.150000
16 Command line string: >> -spacegroup<<
17 Space group set to: P222 (#16)
18 Laue check disabled.
19 Laue group set to: mmm
20 Lattice set to oP
21 Command line string: >> -laueonly<<
22 Laue Check
23 -----------------------------------------------------
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 -----------------------------------------------------
34 Laue Unique axis Num Calc Obs R-Merge Pass?
35 class axis unique mult mult
36 -1 - 1314 1 2.01 0.02 [PASS]
37 2/m a 3786 2 2.25 0.02 [PASS]
38 2/m b 4037 2 2.29 0.02 [PASS]
39 2/m c 1996 2 2.13 0.02 [PASS]
```

CrystalClear User Manual  Page 179
Appendix C: Sample Log Files

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   4/mmm       a    3213     8   3.40      0.44  ----
47   4/mmm       b    2532     8   2.81     0.30  ----
48   4/mmm       c    2732     8   4.10     0.33  ----
49     -3       -    2782     3   2.58     0.59  ----
50     -3m1      -    2979     6   3.23     0.65  ----
51     -3m1      -    3169     6   3.25     0.64  ----
52     -3/m       -    2947     6   3.44     0.53  ----
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 /****************************************************************************
12 Finished reading command line.
13 Input Cell:        [   6.36  15.51  25.07  90.00  90.00  90 .00 ]
14 Input Sigmas:      [ 0.0003 0.0009 0.0013 0.0000 0.0000 0.0000 ]
15 Input Orientation: [  97.41  -1.70 171.25 ]
16 Reading Reflection file dtintegrate.ref ...
17 INFO in Creflnlist::nRead with filename: dtintegrate.ref
18 INFO in Creflnlist::nRead, EOF after 12641 reflections read in
19 (12641 total now in list).
20 N(Z) test: fraction of intensities less than Z x <I>
21 ---------------------------------------------------------------------
22 Z=        0.1    0. 2    0.3    0.4    0.5    0.6    0.7    0.8    0.9    1.0
23 centric   .248   .345   .419   .479   .520   .561   .597   .629   .657   .683
25 deviation -.153  -.164  -.160  -.149  -.126  -.110  -.094  -.078  -.064  -.051
26 theoretical average deviation =>   -.115
27 measured  0.317  0.463  0.556  0.617  0.665  0.698  0.723  0.745  0.766  0.781
28 deviation -0.069 -0.118 -0.137 -0.138 -0.145 -0.137 -0.126 -0.116 -0.109 -0.098
29 measured average deviation =>   -0.119
30 -----------------------------------------------------------------------
31 Centric Distribution Selected.
32 No reindexing done.
33 Reflection file not updated.
34 Header "output.head" written.

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 \n5   -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.
Appendix C: Sample Log Files

Command line string: >>-head<<
Output Header Name set to "output.head".
Command line string: >>-lauegroup<<
Laue group set to: mmm
Laue check disabled.
Command line string: >>-acentric<<
Space group is Acentric.
Centricity check disabled.
Command line string: >>-rejects<<
Command line string: >>-asigma<<
Absence I/Sigma(I) set to 10.000000

Finished reading command line.

Input Cell: [ 6.36 15.51 25.07 90.00 90.00 90.00 ]
Input Sigmas: [ 0.0003 0.0009 0.0013 0.0000 0.0000 0.0000 ]
Input Orientation: [ 97.41 -1.70 171.25 ]

Reading Reflection file dtintegrate.ref ...
Creflnlist::nRead with filename: dtintegrate.ref
INFO in Creflnlist::nRead, EOF after 12641 reflections read in
(12641 total now in list).

Checking systematic absences...
Outputing 'dtcell_rejects.ref'...
Number of reflections written: 3724

BEGIN Texsan Output

Odd/Even parity class
--------------------------------
Class Total Observed <I/sig>
--------------------------------
  eee  1606  1364  160.9  
  eeo  1593  1325  166.6  
  eoe  1576  1295  169.2  
  eoo  1571  1362  174.9  
  oee  1572  1362  164.9  
  oeo  1573  1380  155.4  
  ooe  1572  1378  181.8  
  ooo  1578  1404  181.3  

---------------------------------    --------------------------------
---------------------------------    --------------------------------
  hk0 Total Observed <I/sig>  h0l Total Observed <I/sig>
---------------------------------    --------------------------------
  ee  83  68  367.3  e e  102  79  258.4  
  eo  74  44  222.4  e o  101  62  105.3  
  oe  78  63  296.6  o e  103  85  276.9  
  oo  77  53  250.1  o o  100  80  208.8  

---------------------------------    --------------------------------
---------------------------------    --------------------------------
  0kl Total Observed <I/sig>  hhl Total Observed <I/sig>
---------------------------------    --------------------------------
  ee  374  287  185.4  e e  97  89  380.6  
  eo  372  291  181.9  e o  98  73  357.0  
  oe  354  266  217.1  o e  96  90  378.7  
  oo  360  284  257.4  o o  94  88  434.2  

---------------------------------    --------------------------------
---------------------------------    --------------------------------
  h-hl Total Observed <I/sig>
--------------------------------
  ee  114  98  236.7  
  eo  113  77  183.4  
  oe  113  107  249.9  
  oo  117  108  304.1  

---------------------------------    --------------------------------
---------------------------------    --------------------------------
  hhh Total Observed <I/sig>  hh0 Total Observed <I/sig>
---------------------------------    --------------------------------
  e  5  5  708.6  e  5  3  496.1  
  o  7  7  1008.4  o  5  5  919.9  

CrystalClear User Manual  Page 181
## Appendix C: Sample Log Files

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<td>6327</td>
<td>734</td>
<td>------</td>
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<td>5492</td>
<td>571</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td></td>
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</tr>
<tr>
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<td>170.87</td>
<td>220.72</td>
<td>------</td>
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</tr>
<tr>
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<td>204</td>
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<td></td>
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<tr>
<td></td>
<td>171.94</td>
<td>------</td>
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<td>------</td>
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<td>5399</td>
<td>------</td>
<td>107</td>
<td>------</td>
<td>------</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>166.00</td>
<td>------</td>
<td>260.44</td>
<td>------</td>
<td>------</td>
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<td></td>
</tr>
<tr>
<td>h+k=2n</td>
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<td>160</td>
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<td>5471</td>
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<td>121</td>
<td>------</td>
<td>------</td>
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</tr>
<tr>
<td></td>
<td>173.09</td>
<td>------</td>
<td>310.90</td>
<td>------</td>
<td>------</td>
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</tr>
<tr>
<td>h!=4n</td>
<td>9572</td>
<td>------</td>
<td>310</td>
<td>229</td>
<td>7</td>
<td>------</td>
<td></td>
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<tr>
<td></td>
<td>8376</td>
<td>------</td>
<td>244</td>
<td>172</td>
<td>7</td>
<td>------</td>
<td></td>
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<tr>
<td></td>
<td>175.36</td>
<td>------</td>
<td>239.44</td>
<td>293.55</td>
<td>554.96</td>
<td>------</td>
<td></td>
</tr>
<tr>
<td>h=4n</td>
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<td>------</td>
<td>96</td>
<td>83</td>
<td>1</td>
<td>------</td>
<td></td>
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<tr>
<td></td>
<td>2494</td>
<td>------</td>
<td>62</td>
<td>56</td>
<td>1</td>
<td>------</td>
<td></td>
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<tr>
<td></td>
<td>151.46</td>
<td>------</td>
<td>126.74</td>
<td>266.36</td>
<td>75.42</td>
<td>------</td>
<td></td>
</tr>
<tr>
<td>k!=4n</td>
<td>9469</td>
<td>1097</td>
<td>------</td>
<td>231</td>
<td>------</td>
<td>27</td>
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</tr>
<tr>
<td></td>
<td>8188</td>
<td>842</td>
<td>------</td>
<td>167</td>
<td>------</td>
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<td></td>
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<tr>
<td></td>
<td>176.10</td>
<td>220.86</td>
<td>------</td>
<td>285.36</td>
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<td>311.34</td>
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<tr>
<td>k=4n</td>
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<td>------</td>
<td>81</td>
<td>------</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2682</td>
<td>286</td>
<td>------</td>
<td>61</td>
<td>------</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>150.05</td>
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<td>------</td>
<td>289.04</td>
<td>------</td>
<td>572.17</td>
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<td>l!=4n</td>
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<td>------</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td></td>
<td>8175</td>
<td>857</td>
<td>223</td>
<td>------</td>
<td>------</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>168.43</td>
<td>213.57</td>
<td>210.68</td>
<td>------</td>
<td>------</td>
<td>135.82</td>
<td></td>
</tr>
<tr>
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<td>104</td>
<td>------</td>
<td>------</td>
<td>9</td>
<td></td>
</tr>
</tbody>
</table>
Appendix C: Sample Log Files

<table>
<thead>
<tr>
<th>Refln. Type</th>
<th>hkl</th>
<th>0kl</th>
<th>h0l</th>
<th>hk0</th>
<th>h00</th>
<th>0k0</th>
<th>00l</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Reflns</td>
<td>12641</td>
<td>1460</td>
<td>406</td>
<td>312</td>
<td>8</td>
<td>37</td>
<td></td>
</tr>
<tr>
<td>Condition</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>Num Reflns.</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>18</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>Num Observed</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>&lt;I/sig(I)&gt;</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-0.55</td>
<td>3.01</td>
<td></td>
</tr>
</tbody>
</table>

Sending tcl command

Systematic Absences <I/sig(I)> <= 10.00

<table>
<thead>
<tr>
<th>Refln. Type</th>
<th>hk1</th>
<th>0k1</th>
<th>h01</th>
<th>hk0</th>
<th>h00</th>
<th>0k0</th>
<th>00l</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Reflns</td>
<td>12641</td>
<td>1460</td>
<td>406</td>
<td>312</td>
<td>8</td>
<td>37</td>
<td></td>
</tr>
<tr>
<td>Condition</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>Num Reflns.</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>18</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>Num Observed</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>&lt;I/sig(I)&gt;</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-0.55</td>
<td>3.01</td>
<td></td>
</tr>
</tbody>
</table>

Sending tcl command

Spacegroups found.

Number Name Presentation Centricity Likelihood

| 18  | P21212 | P22121 | Acentric | 1.00 |

Space groups whose 'Presentation' field differs from the 'Name' field were found in a non-standard presentation.
Re-indexing will be required to convert to a standard presentation.

Options:
T) Print Texsan Output
S) Print Selected Spacegroups
A) Print Table of absences used to selected spacegroups
B) Print Table of all absences applicable to laue group
Q) Quit
#) Type spacegroup number.
Enter) Select spacegroup 18

Choice: Q

Terminating.
No reindexing done.
Reflection file not updated.
Header "output.head" written.

Scale and Average Log
Appendix C: Sample Log Files

```
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 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.
```

CrystalClear User Manual  Page 185
Appendix C: Sample Log Files

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

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 $f_{\text{Obs}}_{\text{pixel0}}$ and $f_{\text{Obs}}_{\text{pixel1}}$ fields are in millimeters and not pixels. This table is a quick check that the input reflection list contains the expected range of values.

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.

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.

Lines 99-100  This confirms that you excluded reflections with $I/\sigma \lessgtr 3$ 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.
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.

<table>
<thead>
<tr>
<th></th>
<th>Method 1</th>
<th>Expected $R_{merge}$:</th>
<th>0.033</th>
</tr>
</thead>
<tbody>
<tr>
<td>104</td>
<td>Method 2</td>
<td>Expected $R_{merge}$:</td>
<td>0.034</td>
</tr>
<tr>
<td>105</td>
<td>Actual</td>
<td>$R_{merge}$:</td>
<td>0.032</td>
</tr>
</tbody>
</table>

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

Method 1: \[ R_{merge} = \frac{1}{\sqrt{I_h}} , \text{ where } I_h \text{ is the average intensity for all averaged reflections.} \]

Method 2: \[ R_{merge} = \frac{\sigma_h}{I_h} \sqrt{\frac{N_h}{N_i}} , \text{ where } \sigma_h \text{ is the average standard deviation for averaged reflections, } N_h \text{ is the number of unique reflections, and } N_i \text{ is the number of overlaps.} \]

Actual: \[ R_{merge} = \frac{\sum_h \sum_i |I_{hi} - I_h|}{\sum_h \sum_i |I_h|} \]

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 $R_{merge}$ calculations. A high redundancy will improve the $I/\sigma$ in the merged and averaged results (see e.g. the dtscalemerge documentation Eqn. 10).

<table>
<thead>
<tr>
<th></th>
<th>Multiplicity of observed reflections</th>
</tr>
</thead>
<tbody>
<tr>
<td>107</td>
<td>-------------------------------------</td>
</tr>
<tr>
<td>108</td>
<td>Mult</td>
</tr>
<tr>
<td>110</td>
<td>Refs</td>
</tr>
<tr>
<td>112</td>
<td>Reflections with a multiplicity of 1 are not used in scale factor refinement nor in $R_{merge}$ calculations.</td>
</tr>
</tbody>
</table>

Lines 114-119 Overlaps among scaling batches

<table>
<thead>
<tr>
<th></th>
<th>Overlaps among scaling batches</th>
</tr>
</thead>
<tbody>
<tr>
<td>116</td>
<td>Batch</td>
</tr>
<tr>
<td>118</td>
<td>L001</td>
</tr>
<tr>
<td>119</td>
<td>L002</td>
</tr>
<tr>
<td>120</td>
<td>L003</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
<tr>
<td>163</td>
<td>L020</td>
</tr>
</tbody>
</table>
Appendix C: Sample Log Files

Lines 114-166  Overlaps among the scaling batches are listed next (but only if the dtscalmerge 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 non-linear 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 excruciatingly clear, here is another example: suppose batch X001 has 10 copies of a reflection with $hkl = (1012)$ and batch X002 has just 1 copy. The table will then appear:

<table>
<thead>
<tr>
<th>Batch</th>
<th>X001</th>
<th>X002</th>
</tr>
</thead>
<tbody>
<tr>
<td>X001</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>X002</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

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).

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

<table>
<thead>
<tr>
<th>Batch name</th>
<th>Num refs</th>
<th>Num excluded</th>
<th>Num rejs</th>
<th>Num ovlps</th>
<th>Num singles</th>
</tr>
</thead>
<tbody>
<tr>
<td>L001</td>
<td>1603</td>
<td>206</td>
<td>53</td>
<td>1327</td>
<td>17</td>
</tr>
<tr>
<td>L002</td>
<td>1625</td>
<td>227</td>
<td>40</td>
<td>1341</td>
<td>17</td>
</tr>
<tr>
<td>L003</td>
<td>1609</td>
<td>238</td>
<td>34</td>
<td>1310</td>
<td>27</td>
</tr>
<tr>
<td>L004</td>
<td>1574</td>
<td>238</td>
<td>25</td>
<td>1280</td>
<td>31</td>
</tr>
<tr>
<td>...</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>L020</td>
<td>1590</td>
<td>268</td>
<td>28</td>
<td>1152</td>
<td>142</td>
</tr>
<tr>
<td>All batches</td>
<td>31914</td>
<td>5294</td>
<td>585</td>
<td>25138</td>
<td>897</td>
</tr>
</tbody>
</table>

Num refs Total number of reflections in this batch
Num excluded Number of reflections excluded because of the $I/\sigma$ 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.
Appendix C: Sample Log Files

<table>
<thead>
<tr>
<th>Batch</th>
<th>Num</th>
<th>Scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>name</td>
<td>ovlps</td>
<td>K</td>
</tr>
<tr>
<td>L001</td>
<td>1327</td>
<td>1.0138</td>
</tr>
<tr>
<td>L002</td>
<td>1341</td>
<td>1.0000</td>
</tr>
<tr>
<td>L003</td>
<td>1310</td>
<td>0.9911</td>
</tr>
</tbody>
</table>

... 
| L018  | 1203 | 1.0519 | 0.0000 | -0.3011 | 0.0000 |
| L019  | 1149 | 1.0593 | 0.0000 | -0.3365 | 0.0000 |
| L020  | 1152 | 1.0748 | 0.0000 | -0.3388 | 0.0000 |

*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:

$$ I_{corr} = I_{hi} = I_{hj} \times k_j e^{-2\beta_{hi} sin^2 \theta / \lambda^2} $$

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.

In the tables below Rmerge is defined as:

$$ Rmerge = \frac{\text{Sum Sum} |I_{hi} - <I_h>|}{\text{Sum Sum} <I_h>} $$

where $I_{hi}$ is the $i$th used observation for unique hkl $h$, and $<I_h>$ is the mean intensity for unique hkl $h$.

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

<table>
<thead>
<tr>
<th>Batch</th>
<th>Average</th>
<th>Num</th>
<th>Num</th>
<th>Num</th>
<th>Num</th>
<th>&lt;I/</th>
<th>ChiSq</th>
<th>Rmerge</th>
<th>Rmerge</th>
<th>Rmerge</th>
</tr>
</thead>
<tbody>
<tr>
<td>name</td>
<td>counts</td>
<td>obs</td>
<td>rejs</td>
<td>ovlps</td>
<td>single</td>
<td>sig&gt;</td>
<td>batch</td>
<td>cumul</td>
<td>batch</td>
<td>cumul</td>
</tr>
<tr>
<td>L001</td>
<td>965</td>
<td>1397</td>
<td>53</td>
<td>1327</td>
<td>17</td>
<td>12.4</td>
<td>0.387</td>
<td>0.036</td>
<td>0.036</td>
<td></td>
</tr>
<tr>
<td>L002</td>
<td>997</td>
<td>1398</td>
<td>40</td>
<td>1341</td>
<td>17</td>
<td>15.0</td>
<td>0.425</td>
<td>0.033</td>
<td>0.035</td>
<td></td>
</tr>
<tr>
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<tr>
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<tr>
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<td>26</td>
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<td>0.275</td>
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<tr>
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<td>11.4</td>
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<td>0.032</td>
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<td>23</td>
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<td></td>
</tr>
<tr>
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<td>L017</td>
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<td>1264</td>
<td>62</td>
<td>11.1</td>
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<td>0.032</td>
<td>0.032</td>
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<tr>
<td>L018</td>
<td>929</td>
<td>1314</td>
<td>36</td>
<td>1203</td>
<td>75</td>
<td>11.3</td>
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<td>0.032</td>
<td>0.032</td>
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<tr>
<td>L019</td>
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<td>1149</td>
<td>118</td>
<td>11.0</td>
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<td>0.032</td>
<td></td>
</tr>
<tr>
<td>L020</td>
<td>859</td>
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<td>28</td>
<td>1152</td>
<td>142</td>
<td>11.2</td>
<td>0.271</td>
<td>0.033</td>
<td>0.032</td>
<td></td>
</tr>
</tbody>
</table>
The table lists \textit{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 \textit{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 \textit{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. |
| \textit{<I/sig>} | The average Intensity/SigmaI for reflections in the batch. This is for the corrected but unmerged reflections. A higher \textit{<I/sig>} was expected for the averaged reflections shown in subsequent tables. |
| ChiSq | This is the pseudo-normalized $\chi^2$ for each batch. |
| Rmerge batch | This is the \textit{Rmerge} of the reflections which belong to this batch where $\bar{I}_h$ is calculated from reflections from all batches. |
| Rmerge cumul | This is the \textit{Rmerge} of the reflections which belong to this batch and all previous batches in the table where $\bar{I}_h$ is calculated from reflections from all batches. |

### Table: \textit{Rmerge vs Intensity/SigmaI}

<table>
<thead>
<tr>
<th>Int/sigmaI range</th>
<th>Average counts</th>
<th>Num obs</th>
<th>Num rejs</th>
<th>Num ovlps</th>
<th>Num mults</th>
<th>\textit{&lt;I/sig&gt;}</th>
<th>ChiSq</th>
<th>Rmerge</th>
<th>Rmerge cumul</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 - &gt;20</td>
<td>1470</td>
<td>15510</td>
<td>326</td>
<td>15086</td>
<td>3407</td>
<td>30.9</td>
<td>1.225</td>
<td>0.029</td>
<td>0.029</td>
</tr>
<tr>
<td>16 - 18</td>
<td>271</td>
<td>1567</td>
<td>49</td>
<td>1497</td>
<td>384</td>
<td>16.0</td>
<td>1.133</td>
<td>0.057</td>
<td>0.029</td>
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<tr>
<td>14 - 16</td>
<td>206</td>
<td>1658</td>
<td>39</td>
<td>1584</td>
<td>421</td>
<td>14.0</td>
<td>1.032</td>
<td>0.065</td>
<td>0.030</td>
</tr>
<tr>
<td>12 - 14</td>
<td>160</td>
<td>1713</td>
<td>49</td>
<td>1614</td>
<td>447</td>
<td>12.0</td>
<td>0.939</td>
<td>0.073</td>
<td>0.030</td>
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<tr>
<td>10 - 12</td>
<td>120</td>
<td>1936</td>
<td>46</td>
<td>1857</td>
<td>536</td>
<td>10.0</td>
<td>0.852</td>
<td>0.088</td>
<td>0.031</td>
</tr>
<tr>
<td>8 - 10</td>
<td>94</td>
<td>1648</td>
<td>26</td>
<td>1583</td>
<td>512</td>
<td>8.0</td>
<td>0.601</td>
<td>0.092</td>
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</tr>
<tr>
<td>6 - 8</td>
<td>70</td>
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<td>39</td>
<td>1370</td>
<td>520</td>
<td>6.0</td>
<td>0.416</td>
<td>0.114</td>
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</tr>
<tr>
<td>4 - 6</td>
<td>49</td>
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<td>11</td>
<td>547</td>
<td>263</td>
<td>4.9</td>
<td>0.188</td>
<td>0.117</td>
<td>0.032</td>
</tr>
<tr>
<td>&lt; 0 - 2</td>
<td>---</td>
<td>274</td>
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<td>0</td>
<td>3</td>
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<td>---</td>
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</tr>
<tr>
<td>&lt; 0</td>
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<td>0</td>
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<td>0.032</td>
</tr>
</tbody>
</table>

### Table: \textit{Rmerge vs Intensity/SigmaI}

<table>
<thead>
<tr>
<th>Int/sigmaI range</th>
<th>Average counts</th>
<th>Num obs</th>
<th>Num rejs</th>
<th>Num ovlps</th>
<th>Num mults</th>
<th>\textit{&lt;I/sig&gt;}</th>
<th>ChiSq</th>
<th>Rmerge</th>
<th>Rmerge cumul</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 - &gt;20</td>
<td>941</td>
<td>26620</td>
<td>585</td>
<td>25138</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td>0.032</td>
</tr>
<tr>
<td>16 - 18</td>
<td>26620</td>
<td>585</td>
<td>25138</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td>0.032</td>
<td>0.032</td>
</tr>
<tr>
<td>14 - 16</td>
<td>25138</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12 - 14</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 - 12</td>
<td>26620</td>
<td>585</td>
<td>25138</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td>0.032</td>
<td>0.032</td>
</tr>
<tr>
<td>8 - 10</td>
<td>585</td>
<td>25138</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6 - 8</td>
<td>25138</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 - 6</td>
<td>897</td>
<td>12.0</td>
<td>0.29</td>
<td>0.032</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>&lt; 0 - 2</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>0.032</td>
</tr>
<tr>
<td>&lt; 0</td>
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<td>0</td>
<td>0</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>0.032</td>
</tr>
</tbody>
</table>

Lines 226-252 This table lists \textit{Rmerge vs Batch}. It is easy to recognize any batch not matching well with the other batches.
### Appendix C: Sample Log Files

<table>
<thead>
<tr>
<th>Description</th>
<th>Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average counts</td>
<td>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 $R_{\text{merge}}$ for this shell would be $1/\sqrt{I}$. So, for the shell of highest $I/\sigma$, $1/\sqrt{1470} = 0.026$ is consistent with 0.029 found. In the 4-6 shell, $1/\sqrt{49} = 0.142$ is consistent with 0.117 found.</td>
</tr>
<tr>
<td>Num obs</td>
<td>Number of reflections in this shell.</td>
</tr>
<tr>
<td>Num rejs</td>
<td>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.</td>
</tr>
<tr>
<td>Num ovlps</td>
<td>Number of reflections in this shell having symmetry-related mates and that contributed to the $R_{\text{merge}}$.</td>
</tr>
<tr>
<td>Num mults</td>
<td>Number of unique reflections measured multiple times in the shell. The average multiplicity or redundancy for the shell is Num ovlps / Num mults.</td>
</tr>
<tr>
<td>$&lt;I/\sigma&gt;$</td>
<td>The average Intensity/Signal for averaged reflections in the shell. As expected, there is a larger $&lt;I/\sigma&gt;$ for the averaged reflections than shown for unaveraged reflections in the $R_{\text{merge}}$ vs. Batch table.</td>
</tr>
<tr>
<td>ChiSq norm</td>
<td>This is the normalized $\chi^2$ popularized by Dr. Zbyszek Otwinowski calculated as $\chi^2 = \frac{1}{(N_{hi} - N_h)} \sum_{h} \sum_{i} W_{hi} (I_{hi} - \bar{I}<em>h)^2$ where $N_h$ is the number of unique reflections and $N</em>{hi}$ is the number of contributors to or multiplicity of averaged reflection $\bar{I}<em>h$. Values close to 1 suggest that the error model ($w</em>{hi}$) is valid.</td>
</tr>
<tr>
<td>$R_{\text{merge}}$ shell</td>
<td>This is the $R_{\text{merge}}$ for reflections which belong to this shell.</td>
</tr>
<tr>
<td>$R_{\text{merge}}$ cumul</td>
<td>This is the cumulative $R_{\text{merge}}$ for reflections which belong to this shell and all previous shells. It shows what the $R_{\text{merge}}$ would be if the data is cut off at different $I/\sigma$ levels.</td>
</tr>
</tbody>
</table>

Remark: Use the table to determine at what resolution the crystal stopped diffracting.
### Appendix C: Sample Log Files

**270** Rmerge vs Resolution

<table>
<thead>
<tr>
<th>Resolution range</th>
<th>Average counts</th>
<th>Num obs</th>
<th>Num rejs</th>
<th>Num ovlps</th>
<th>Num mults</th>
<th>&lt;I/sig&gt; norm</th>
<th>ChiSq norm</th>
<th>Rmerge shell</th>
<th>Rmerge cumul</th>
</tr>
</thead>
<tbody>
<tr>
<td>79.2 - 6.12</td>
<td>2260</td>
<td>278</td>
<td>31</td>
<td>228</td>
<td>64</td>
<td>21.2</td>
<td>0.797</td>
<td>0.042</td>
<td>0.042</td>
</tr>
<tr>
<td>6.12 - 4.34</td>
<td>2346</td>
<td>1564</td>
<td>44</td>
<td>1468</td>
<td>351</td>
<td>28.2</td>
<td>0.945</td>
<td>0.029</td>
<td>0.031</td>
</tr>
<tr>
<td>4.34 - 3.54</td>
<td>3147</td>
<td>2196</td>
<td>37</td>
<td>2095</td>
<td>492</td>
<td>33.7</td>
<td>0.934</td>
<td>0.024</td>
<td>0.027</td>
</tr>
<tr>
<td>3.54 - 3.07</td>
<td>2102</td>
<td>2586</td>
<td>39</td>
<td>2482</td>
<td>603</td>
<td>32.0</td>
<td>1.014</td>
<td>0.026</td>
<td>0.026</td>
</tr>
<tr>
<td>3.07 - 2.74</td>
<td>1055</td>
<td>2963</td>
<td>55</td>
<td>2836</td>
<td>705</td>
<td>27.5</td>
<td>1.086</td>
<td>0.030</td>
<td>0.027</td>
</tr>
<tr>
<td>2.74 - 2.51</td>
<td>597</td>
<td>3137</td>
<td>69</td>
<td>2982</td>
<td>747</td>
<td>22.7</td>
<td>1.125</td>
<td>0.036</td>
<td>0.028</td>
</tr>
<tr>
<td>2.51 - 2.32</td>
<td>382</td>
<td>3321</td>
<td>74</td>
<td>3170</td>
<td>834</td>
<td>17.6</td>
<td>0.999</td>
<td>0.045</td>
<td>0.029</td>
</tr>
<tr>
<td>2.32 - 2.17</td>
<td>278</td>
<td>3378</td>
<td>76</td>
<td>3199</td>
<td>832</td>
<td>14.0</td>
<td>1.028</td>
<td>0.057</td>
<td>0.030</td>
</tr>
<tr>
<td>2.17 - 2.05</td>
<td>192</td>
<td>3204</td>
<td>72</td>
<td>3002</td>
<td>813</td>
<td>11.0</td>
<td>0.999</td>
<td>0.071</td>
<td>0.031</td>
</tr>
<tr>
<td>2.05 - 1.94</td>
<td>118</td>
<td>3993</td>
<td>88</td>
<td>3676</td>
<td>1049</td>
<td>8.4</td>
<td>0.890</td>
<td>0.090</td>
<td>0.032</td>
</tr>
<tr>
<td>1.94 - 1.92</td>
<td>941</td>
<td>26620</td>
<td>585</td>
<td>25138</td>
<td>6490</td>
<td>19.5</td>
<td>1.000</td>
<td>0.032</td>
<td>0.032</td>
</tr>
</tbody>
</table>

**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 \(1/\sqrt{I}\). So for the shell of highest \(I/\sigma\),

\[
1/\sqrt{2260} = 0.021
\]

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,

\[
1/\sqrt{118} = 0.092
\]

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 \(\chi^2\) 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.
### Completeness vs Resolution

<table>
<thead>
<tr>
<th>Resolution range</th>
<th>Calc unique</th>
<th>Num obs</th>
<th>Num rejs</th>
<th>Num mults</th>
<th>Num single</th>
<th>Num unique</th>
<th>Avg mult</th>
<th>%Comp shell</th>
<th>%Comp cumul</th>
</tr>
</thead>
<tbody>
<tr>
<td>79.2 - 6.12</td>
<td>363</td>
<td>278</td>
<td>31</td>
<td>64</td>
<td>83</td>
<td>2.98</td>
<td>22.9</td>
<td>22.9</td>
<td></td>
</tr>
<tr>
<td>6.12 - 4.34</td>
<td>593</td>
<td>1564</td>
<td>44</td>
<td>351</td>
<td>52</td>
<td>403</td>
<td>3.77</td>
<td>68.0</td>
<td>50.8</td>
</tr>
<tr>
<td>4.34 - 3.54</td>
<td>736</td>
<td>2196</td>
<td>37</td>
<td>492</td>
<td>64</td>
<td>556</td>
<td>3.88</td>
<td>75.5</td>
<td>61.6</td>
</tr>
<tr>
<td>3.54 - 3.07</td>
<td>863</td>
<td>2586</td>
<td>39</td>
<td>603</td>
<td>65</td>
<td>668</td>
<td>3.81</td>
<td>77.4</td>
<td>66.9</td>
</tr>
<tr>
<td>3.07 - 2.74</td>
<td>966</td>
<td>2963</td>
<td>55</td>
<td>705</td>
<td>72</td>
<td>777</td>
<td>3.74</td>
<td>80.4</td>
<td>70.6</td>
</tr>
<tr>
<td>2.74 - 2.51</td>
<td>1061</td>
<td>3137</td>
<td>69</td>
<td>747</td>
<td>86</td>
<td>833</td>
<td>3.68</td>
<td>78.5</td>
<td>72.5</td>
</tr>
<tr>
<td>2.51 - 2.32</td>
<td>1131</td>
<td>3321</td>
<td>74</td>
<td>834</td>
<td>77</td>
<td>911</td>
<td>3.56</td>
<td>80.5</td>
<td>74.1</td>
</tr>
<tr>
<td>2.32 - 2.17</td>
<td>1226</td>
<td>3378</td>
<td>76</td>
<td>832</td>
<td>103</td>
<td>935</td>
<td>3.53</td>
<td>76.3</td>
<td>74.4</td>
</tr>
<tr>
<td>2.17 - 2.05</td>
<td>1290</td>
<td>3204</td>
<td>72</td>
<td>813</td>
<td>130</td>
<td>943</td>
<td>3.32</td>
<td>73.1</td>
<td>74.2</td>
</tr>
<tr>
<td>2.05 - 1.94</td>
<td>1362</td>
<td>3993</td>
<td>88</td>
<td>1049</td>
<td>229</td>
<td>1278</td>
<td>3.06</td>
<td>93.8</td>
<td>77.0</td>
</tr>
<tr>
<td>1.94 - 1.79</td>
<td>9591</td>
<td>26620</td>
<td>585</td>
<td>6490</td>
<td>897</td>
<td>7387</td>
<td>3.52</td>
<td>77.0</td>
<td>77.0</td>
</tr>
</tbody>
</table>

**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.
Appendix C: Sample Log Files

Direct Beam Log

A summary of the typical log file DirectBeam.log generated by the direct beam shot utility is shown below.

```
Direct Beam Utility  Copyright (c) 1998 Molecular Structure Corporation
Number of cycles: 5
Exposure time: 1 seconds
Date: Thu Mar 30 16:41:19 2000

.................
.................
.................
.......111111.....
.....111111111....
....11222222211....
.....112333333211....
......1123456543211....
....11223579A9753211....
....112357ADFFB85311....
...112357AFJNMB63211... Direct beam for IP 1, cycle 1
..112469DJQTN8421... Position (x,y) = (1499.84, 1509.80)
..11247AFMUZXQG95211... Pixel Intensity = 10841
..11247BGOV+YQG95211... Integrated Intensity, sigma(I) = 330647, 895
..11246AGMTXVNF8421... I/sigma(I) = 369.5
..112358DIORQKC7321... 3sigma width (x,y) = (12, 13)
..112469DHJJE95311... Full width at half maximum (x,y) = (5.57, 6.86)
...123469BDDA7421....
...11234578875321....
....1122345553211....
.....112233333211.....
.......11111222111....
..............11111....
.................
.................
.................

Average direct beam results for IP 1
Position (x,y) = (1499.64, 1509.61) +/- (0.262854, 0.14148)
Pixel Intensity = 10533 +/- 445.806
Integrated Intensity, sigma(I) = 336594, 893.455 +/- (4324.93, 4.73774)
I/sigma(I) = 376.732 +/- 4.30341
Full width at half maximum (x,y) = (5.55258, 6.88398) +/- (0.0486711, 0.0397825)
```
Appendix C: Sample Log Files

Average direct beam results for IP 2
Position (x,y) = (1500.92, 1509.61) +/- (0.266244, 0.175193)
Pixel Intensity = 10740.4 +/- 268.098
Integrated Intensity, sigma(I) = 336789, 896.288 +/- (4495.92, 3.81553)
I/sigma(I) = 375.777 +/- 6.19005
Full width at half maximum (x,y) = (5.57419, 6.89354) +/-
(0.0479199, 0.0299656)

<table>
<thead>
<tr>
<th>Cycle</th>
<th>IP1</th>
<th>IP2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>x</td>
<td>y</td>
</tr>
<tr>
<td>1</td>
<td>1499.8</td>
<td>1509.8</td>
</tr>
<tr>
<td>2</td>
<td>1499.4</td>
<td>1509.6</td>
</tr>
<tr>
<td>3</td>
<td>1499.4</td>
<td>1509.4</td>
</tr>
<tr>
<td>4</td>
<td>1499.6</td>
<td>1509.7</td>
</tr>
<tr>
<td>5</td>
<td>1500.0</td>
<td>1509.5</td>
</tr>
</tbody>
</table>

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.

Direct Beam Utility
Number of cycles: 1
Exposure time: 1.0 seconds
Date: Thu Sep 30 17:34:19 1999
Average direct beam position for IP1 = (2682.6, 1505.9)
Average direct beam position for IP2 = (2683.5, 1505.5)

<table>
<thead>
<tr>
<th>Cycle</th>
<th>IP1</th>
<th>IP2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>x</td>
<td>y</td>
</tr>
</tbody>
</table>
Appendix C: Sample Log Files

---

1     2682.6, 1505.9 [ 7090]   2683.5, 1505.5 [ 7209]

Direct Beam Utility
Number of cycles: 2
Exposure time: 1.0 seconds
Date: Tue Oct 19 11:02:31 1999

Average direct beam position for IP1 = (1505.1,1506.6)
Average direct beam position for IP2 = (1507.1,1506.7)

IP1                       IP2
Cycle      x       y       I         x       y       I
-----   -----------------------   -----------------------
 1     1504.2, 1507.0 [241280]   1506.2, 1506.8 [247008]
 2     1506.1, 1506.3 [ 14490]   1508.0, 1506.7 [ 14340]
...

Direct Beam Utility
Number of cycles: 5
Exposure time: 1.0 seconds
Date: Thu Mar 30 16:56:17 2000

Average direct beam position for IP1 = (1499.6,1509.6)
Average direct beam position for IP2 = (1500.9,1509.6)

IP1                       IP2
Cycle      x       y       I         x       y       I
-----   -----------------------   -----------------------
 1     1499.8, 1509.8 [ 10841]   1500.7, 1509.8 [ 10932]
 2     1499.4, 1509.6 [ 10346]   1501.3, 1509.4 [ 10267]
 3     1499.4, 1509.4 [  9872]   1501.0, 1509.7 [ 10826]
 4     1499.6, 1509.7 [ 11006]   1500.9, 1509.5 [ 10846]
 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.

---

PMT Check Utility Copyright (c) 1998,1999 Molecular Structure Corporation
Date: Wed Apr 05 15:52:11 2000
Appendix C: Sample Log Files

Result of PMT Test:

- Average = 5.5770
- 3*Sigma = 1.8184
- 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.

PMT Check Utility
Date: Wed Jan 05 12:21:51 2000

Result of PMT Test:
- Average = 6.354
- 3*Sigma = 1.623
- Number of 0 pixels = 0/252000

PMT Check Utility
Date: Wed Apr 05 15:52:11 2000

Result of PMT Test:
- Average = 5.5770
- 3*Sigma = 1.8184
- 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.

Continuous IP Read Utility Copyright (c) 1998 Molecular Structure Corporation
Date: Thu Feb 10 12:19:01 2000

Continuous IP Read test[1/100] => OK Error count = 0
Continuous IP Read test[2/100] => OK Error count = 0
Continuous IP Read test[3/100] => OK Error count = 0
Continuous IP Read test[4/100] => OK Error count = 0
...
Continuous IP Read test[100/100] => OK Error count = 0

Results of Continuous IP Read test:
## Appendix C: Sample Log Files

<table>
<thead>
<tr>
<th>Number of Cycles</th>
<th>Read Failures</th>
<th>Write Failures</th>
<th>Other Failures</th>
<th>Total Failures</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

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.

```
Continuous IP Read Utility
Date: Thu Oct 07 11:51:04 1999

Results of Continuous IP Read test:
<table>
<thead>
<tr>
<th>Number of Cycles</th>
<th>Read Failures</th>
<th>Write Failures</th>
<th>Other Failures</th>
<th>Total Failures</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Continuous IP Read Utility
Date: Thu Feb 10 12:19:01 2000

Results of Continuous IP Read test:
<table>
<thead>
<tr>
<th>Number of Cycles</th>
<th>Read Failures</th>
<th>Write Failures</th>
<th>Other Failures</th>
<th>Total Failures</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
```

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

<table>
<thead>
<tr>
<th>Problem</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>CrystalClear</em> does not communicate correctly with the X-ray detector on a Windows 95 machine.</td>
<td><em>CrystalClear</em> 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 <em>CrystalClear</em> directory. Make sure the detector is set up correctly.</td>
</tr>
<tr>
<td>When I start <em>CrystalClear</em>, only the menus are displayed. I do not see a full <em>CrystalClear</em> window – only the task bar.</td>
<td><em>CrystalClear</em> was closed while it was minimized. After logging into <em>CrystalClear</em> and selecting the project/sample, right-click <em>CrystalClear</em> on the task bar and select <strong>Maximize</strong>. Close CrystalClear while it is maximized. Open <em>CrystalClear</em> and log in. Now you can reshape the <em>CrystalClear</em> window.</td>
</tr>
<tr>
<td>You attempt to select a processing algorithm, such as d*TREK, PROCESS, or TwinSolve, and you receive the following message: &quot;You must have a sample open to set processing algorithms.&quot;</td>
<td>You must have a sample open before you can select a processing algorithm. Click <strong>File &gt; Open Sample</strong> from the menu to select a sample, or <strong>File &gt; New Sample</strong> to create a new sample.</td>
</tr>
<tr>
<td>The TwinSolve button is grayed out on the Toolbar.</td>
<td>TwinSolve is only available with the Mercury CCD.</td>
</tr>
<tr>
<td>You wish to process data, but the selections on the flow bar do not include processing options.</td>
<td>You have a Collection task selected. From the Task drop down, select a task that includes processing, such as the Process task.</td>
</tr>
<tr>
<td>The settings shown in a dialog have reverted back to the defaults, instead of to settings you specified in a previous session.</td>
<td>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.</td>
</tr>
<tr>
<td><em>CrystalClear</em> takes a long time to respond, then an error message occurs saying that <em>CrystalClear</em> cannot get a response from the RAXIS.</td>
<td>If you are not actually connected to an X-ray detector, you should make sure <em>CrystalClear</em> is set in Simulator mode. Click <strong>Tools &gt; Preferences</strong>, then click the Server tab. Check the detector in the list to force <em>CrystalClear</em> to run in Simulator mode.</td>
</tr>
<tr>
<td>When you attempt a step that requires communication with the CCD Camera, CrystalClear</td>
<td>Open system.configuration, which is found in the <em>CrystalClear</em> directory, and change the value of &quot;DaemonIP&quot; to be the IP address of the computer on which the Rigaku Daemon is running. 9 This solution</td>
</tr>
</tbody>
</table>
### Appendix D: Troubleshooting

<table>
<thead>
<tr>
<th>Hangs.</th>
<th>Applies if MSCServDetCCD.exe or MSCServDetCCD_Simulator.exe is started before the hang occurs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>You installed <em>CrystalClear</em> 1.2 over a 1.1 version, and now your user list is empty.</td>
<td>Your data is not removed when you uninstall or reinstall, so you can just recreate the users in <em>CrystalClear</em>, 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 <strong>Data</strong> field.</td>
</tr>
<tr>
<td>You receive an error when attempting to run <em>CrystalClear</em>: &quot;A required DLL file WS2_32.DLL was not found.&quot;</td>
<td>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 <em>CrystalClear</em> 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.</td>
</tr>
</tbody>
</table>

### Crypto-Box Messages

<table>
<thead>
<tr>
<th>Problem</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crypto-Box Error 8: no dongle found.</td>
<td>The <em>CrystalClear</em> Crypto-Box dongle was not found. Install the dongle and try again.</td>
</tr>
<tr>
<td>Crypto-Box Error 30: Error, the attached Crypto-Box did not come from MSC.</td>
<td>A Crypto-Box was found but it was not issued by MSC. The dongle that came with <em>CrystalClear</em> should be installed on the PC on which <em>CrystalClear</em> is installed.</td>
</tr>
<tr>
<td>Crypto-Box Error 31: Error, registration key in the registry and registration key in the Crypto-Box do not match.</td>
<td>Normally this is caused when <em>CrystalClear</em> was installed with an incorrect license number. In this case, reinstall <em>CrystalClear</em> and input the correct license number during installation. This error can also occur if a non-<em>CrystalClear</em> Crypto-Box dongle is found on the PC, but the <em>CrystalClear</em> dongle was not. In this case, install the <em>CrystalClear</em> Crypto-Box and <em>Crypto-Serv</em> software on the PC, then click the <strong>Check Again</strong> button.</td>
</tr>
</tbody>
</table>
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 left-hand sides of the equation:

\[
I_i A_i = \frac{\sum_{j=1}^{k} w_j I_j A_0^j}{\sum_j w_j}
\]

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 \( A_i^0 \) represents an initial estimate of the absorbance. As implemented in the program the initial \( A_i^0 \) values correspond to that of the spherical crystal; when a new absorption surface is obtained, these replace the original \( A_i^0 \) 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.

\[
A = e^{-\alpha t} = e^{-\beta (r_s + t_i)} = A_p \cdot A_s
\]

These absorbances could also be expanded in a Taylor series,

\[
A = A^0 + \sum_{j} \frac{\partial A}{\partial p_j} \Delta p_j + \text{higher order terms}
\]

If the usual approximation is made of assuming that the higher order contributions are negligible, then by a least squares approach, the \( \Delta p_j \) 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:

\[
A(\phi, \nu) = a_0 + \sum_{l=1}^{8} \sum_{m=-l}^{l} a_{lm} y_{lm}(\phi, \nu)
\]

---

where \( a_{lm} \) represents the coefficients to be determined by refinement and \( y_{lm} \) are the corresponding spherical harmonics, and \( \phi \) and \( \upsilon \) are the equatorial and azimuthal angles of the diffracted x-ray beam, respectively.

An alternate analytic function employs a Fourier series to represent absorbance:

\[
A(\phi_p, \phi_s, \upsilon_p, \upsilon_s) = Q_0 + \sum_{n=0}^{n_{\text{max}}} \sum_{m=0}^{m_{\text{max}}} P_{nm} \left( \sin( n\phi_p + m\upsilon_p ) + \sin( n\phi_s + m\upsilon_s ) \right) + Q_{nm} \left( \cos( n\phi_p + m\upsilon_p ) + \cos( n\phi_s + m\upsilon_s ) \right)
\]

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.

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 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.

---

Appendix E: Absorption in Scaling

Table 1. Absorption options

<table>
<thead>
<tr>
<th>Option</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fourier</td>
<td>This option uses Fourier coefficients to model diffracted beam absorption and simple batch scaling to model incident beam absorption, decay, etc.</td>
</tr>
<tr>
<td>4\textsuperscript{th} 3D + 3\textsuperscript{rd} 2D</td>
<td>This option uses 4\textsuperscript{th} order even and odd spherical harmonics to describe the diffracted beam absorption and 3\textsuperscript{rd} order even and odd circular harmonics to model incident beam absorption.</td>
</tr>
<tr>
<td>3\textsuperscript{rd} 3D + 2\textsuperscript{nd} 2D</td>
<td>This option uses 3\textsuperscript{rd} order even and odd spherical harmonics to describe the diffracted beam absorption and 2\textsuperscript{nd} order even and odd circular harmonics to model incident beam absorption.</td>
</tr>
</tbody>
</table>

Table 2. Absorption correction trouble shooting guide.

<table>
<thead>
<tr>
<th>Error Message</th>
<th>Cause and remedy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of outliers exceeds 2000</td>
<td>1. The assumed symmetry is too high. Use “Data analysis -&gt; Laue Group” to automatically determine the Laue group and rerun. 2. The sample is a strong absorber, $\mu R &gt; 2$. 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.</td>
</tr>
<tr>
<td>No convergence in SVDCMP</td>
<td>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 $\theta$ or $\phi$. 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.</td>
</tr>
<tr>
<td>Spherical harmonics methods do not complete</td>
<td>$S \cdot \text{Del}^2 &gt; 10^6$ 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.</td>
</tr>
<tr>
<td>Fourier methods do not complete</td>
<td>$S \cdot \text{Del}^2 &gt; 10^6$ 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.</td>
</tr>
</tbody>
</table>
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: $Zn_{13} = Zn \neq Zn_{cub}$. If the user creates a new sample $Zn_{14}$, its defaults will be identical to $Zn$. Thus: $Zn_{13} = Zn_{14} = Zn \neq Zn_{cub}$.

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

CrystalClear User Manual  Page 205
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 site-level 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

<table>
<thead>
<tr>
<th></th>
<th>RAXIS</th>
<th>Jupiter</th>
<th>Mercury</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Setup</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Crystal To Detector Distance</td>
<td>120</td>
<td>80</td>
<td>50</td>
</tr>
<tr>
<td>2-theta</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Crystal 1 unit cell</td>
<td>80 90 100 90 90 90</td>
<td>80 90 100 90 90 90</td>
<td>10 10 10 90 90 90</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.2 0.2 0.2</td>
<td>0.2 0.2 0.2</td>
<td>0.2 0.2 0.2</td>
</tr>
<tr>
<td>Mosaicity</td>
<td>0.6</td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>Color</td>
<td>Colorless</td>
<td>Colorless</td>
<td>Colorless</td>
</tr>
<tr>
<td>Mount</td>
<td>Loop</td>
<td>Loop</td>
<td>Fiber</td>
</tr>
<tr>
<td>Morphology</td>
<td>Prism</td>
<td>Prism</td>
<td>Prism</td>
</tr>
<tr>
<td>Crystal 2</td>
<td>Unknown</td>
<td>Unknown</td>
<td>Unknown</td>
</tr>
<tr>
<td>Orientation</td>
<td>0 0 0</td>
<td>0 0 0</td>
<td>0 0 0</td>
</tr>
<tr>
<td>Detector Translation</td>
<td>0 0 120</td>
<td>0 0 120</td>
<td>0 0 50</td>
</tr>
<tr>
<td>Rotations</td>
<td>0 0 0</td>
<td>0 0 0</td>
<td>0 0 0</td>
</tr>
<tr>
<td>X-ray Source</td>
<td>50kV 100mA</td>
<td>50kV 100mA</td>
<td>50mV 40mA</td>
</tr>
<tr>
<td>Optics</td>
<td>Copper 1.5418</td>
<td>Copper 1.5418</td>
<td>Molybdenum 0.71073</td>
</tr>
<tr>
<td>Focus</td>
<td>0.3</td>
<td>0.3</td>
<td>1.0</td>
</tr>
<tr>
<td>Collimator</td>
<td>0.3</td>
<td>0.3</td>
<td>0.5</td>
</tr>
<tr>
<td><strong>Initial images</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Images</td>
<td>1 scan of 2 images at</td>
<td>1 scan of 2 images at</td>
<td>4 scans of 1 image at</td>
</tr>
</tbody>
</table>
## Appendix F: Defaults in CrystalClear

<table>
<thead>
<tr>
<th></th>
<th>0, 90 degrees</th>
<th>0, 90 degrees</th>
<th>0, 30, 60, 90 degrees</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Readout</strong></td>
<td>Full frames</td>
<td>Full frames</td>
<td>Full frames</td>
</tr>
<tr>
<td><strong>Exposure</strong></td>
<td>2 min/image</td>
<td>2 min/image</td>
<td>5 sec/image</td>
</tr>
<tr>
<td><strong>Pixel resolution</strong></td>
<td>100 um pixel</td>
<td>2x2 binned</td>
<td>2x2 binned</td>
</tr>
</tbody>
</table>

### Find

<table>
<thead>
<tr>
<th></th>
<th>First image of screen</th>
<th>1-2 of screen</th>
<th>1-4 of screen</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>I/sigma level</strong></td>
<td>3 sigma</td>
<td>3 sigma</td>
<td>3 sigma</td>
</tr>
<tr>
<td><strong>Min pixel</strong></td>
<td>50</td>
<td>50</td>
<td>20</td>
</tr>
<tr>
<td><strong>Peak filter</strong></td>
<td>6</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td><strong>Box</strong></td>
<td>0 0</td>
<td>0 0</td>
<td>0 0</td>
</tr>
<tr>
<td><strong>2D/3D</strong></td>
<td>2D</td>
<td>2D</td>
<td>3D</td>
</tr>
<tr>
<td><strong>Resolution</strong></td>
<td>0 0</td>
<td>0 0</td>
<td>0 0</td>
</tr>
</tbody>
</table>

### Index

<table>
<thead>
<tr>
<th></th>
<th>Unknown</th>
<th>Unknown</th>
<th>Unknown</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>User chooses solution</strong></td>
<td>Yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td><strong>Reflection file</strong></td>
<td>dtfind.ref</td>
<td>dtfind.ref</td>
<td>dtfind.ref</td>
</tr>
<tr>
<td><strong>Max residual</strong></td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td><strong>Indexing method</strong></td>
<td>1D FFT</td>
<td>1D FFT</td>
<td>1D FFT</td>
</tr>
</tbody>
</table>

### Refine

<table>
<thead>
<tr>
<th></th>
<th>0 0</th>
<th>0 0</th>
<th>0 0</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cycles</strong></td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td><strong>I/sig</strong></td>
<td>0</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td><strong>Rejection limits</strong></td>
<td>1 1 2</td>
<td>1 1 2</td>
<td>1 1 2</td>
</tr>
<tr>
<td><strong>Macro</strong></td>
<td>All</td>
<td>All</td>
<td>All</td>
</tr>
</tbody>
</table>

### Predict

<table>
<thead>
<tr>
<th></th>
<th>First image of first scan, screen images unless collect images are available</th>
<th>1-10 of collected images</th>
<th>1-10 of collected images</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Images</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Mosaicity</strong></td>
<td>0.6 unless refined</td>
<td>0.6 unless refined</td>
<td>0.6 unless refined</td>
</tr>
</tbody>
</table>

### Strategy

<table>
<thead>
<tr>
<th></th>
<th>99</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Per cent completeness</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Resolution</strong></td>
<td>0 0</td>
</tr>
<tr>
<td><strong>Speed</strong></td>
<td>Very fast</td>
</tr>
<tr>
<td><strong>Result Limit</strong></td>
<td>360</td>
</tr>
<tr>
<td><strong>Search Rotation</strong></td>
<td>0 360</td>
</tr>
</tbody>
</table>

### Collect

<table>
<thead>
<tr>
<th></th>
<th>2 min RAXISIV++</th>
<th>4 min RAXIS IV</th>
<th>8 min RAXIS II</th>
<th>10-20 sec, sample dependant</th>
<th>20-30 sec, sample dependant</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Exposure time</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Pixel resolution</strong></td>
<td>100 um pixel</td>
<td>2x2 binned</td>
<td>2x2 binned</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Readout</strong></td>
<td>Full</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Integration

<table>
<thead>
<tr>
<th></th>
<th>All collection images</th>
<th>All collection images</th>
<th>All collection images</th>
</tr>
</thead>
</table>
## Appendix F: Defaults in CrystalClear

<table>
<thead>
<tr>
<th><strong>Images per batch</strong></th>
<th>4</th>
<th>4</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Padding</strong></td>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td><strong>Pre-refinement</strong></td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td><strong>Resolution</strong></td>
<td>0 0</td>
<td>0 0</td>
<td>0 0</td>
</tr>
<tr>
<td><strong>Box</strong></td>
<td>0 0, user sets</td>
<td>0 0, user sets</td>
<td>0 0, user sets</td>
</tr>
<tr>
<td><strong>Refinement macro</strong></td>
<td>All</td>
<td>All</td>
<td>All</td>
</tr>
<tr>
<td><strong>Peak radius min/max</strong></td>
<td>3/0</td>
<td>3/0</td>
<td>2/0</td>
</tr>
</tbody>
</table>

### Laue
- **Reflection file**: dtprofit.ref, Dtp roasted.ref, dtintegrate.ref
- **Residual**: 0.15, 0.15, 0.15

### Centricity
- **Reflection file**: dtprofit.ref, Dtp roasted.ref, dtintegrate.ref

### Spacegroup
- **Reflection file**: dtprofit.ref, Dtp roasted.ref, dtintegrate.ref
- **I/sig**: 4, 4, 10

### Scale and Average
- **Reflection file**: dtprofit.ref, Dtp roasted.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
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.

<table>
<thead>
<tr>
<th>Problem</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>The crystal to detector distance is not editable…it states “Per Scan”</td>
<td>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.</td>
</tr>
<tr>
<td>I started a sample as a Process task and the crystal to detector distance shows “0”.</td>
<td>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.</td>
</tr>
<tr>
<td>How do I change the resolution ranges for all steps in processing</td>
<td>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”.</td>
</tr>
<tr>
<td>You have no idea what the cell lengths may be.</td>
<td>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.</td>
</tr>
<tr>
<td>The red plus sign is not in the beam stop shadow</td>
<td>You are collecting images with an improper direct beam position and should contact your administrator to redo direct beam shots.</td>
</tr>
<tr>
<td>I got the “Find Spots Failed” message and the log file shows “…reading image lys0001.osc... Error opening file lys0001.osc Error is: -2”</td>
<td>The image is not there or is corrupted. Wait for the image read to finish.</td>
</tr>
<tr>
<td>Find only found a few spots.</td>
<td>1. Decrease the I/sigma  2. Widen the resolution range 3. Decrease the minimum pixel value 4. Decrease the peak filter.</td>
</tr>
<tr>
<td>Find Spots found too many</td>
<td>1. Slide the number of spots slide in the image information window</td>
</tr>
</tbody>
</table>
## Appendix G: Crystallographic Troubleshooting

<table>
<thead>
<tr>
<th>Issue</th>
<th>Solution</th>
</tr>
</thead>
</table>
| 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 verification.  
|                                                                    | 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 un-check 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 |
| 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. | still have good data which is usable for a first reflection file. |
Index

C

Close the Current Sample · 96
Collect Image · 31
Collect Images
  Mercury CCD · 60
Collect Schedule
  Create · 125, 126
  Delete · 129
  Import · 127
  Run · 128
  Save · 127
Command Bar · 25
Control the Detector · 108
Create a New Processing State · 100
Create a New Sample · 94
Creating a New Project and Sample · 93
Creating Your First Project and Sample · 28
Crypto-Box · 15, 27, 137, 200
Crystallographic Troubleshooting · See Troubleshooting
Current sample · 21

D

d*TREK · 23, 25, 49, 63, 83, 89, 92, 119, 151, 161, 178, 199
Decision Point · 25
Defaults in CrystalClear · See Defaults
Delete Projects and Samples · 97
Dialog Defaults · See Defaults: Dialog
Display Instrument State · 107
Display Processing State · 98
Display Scan State · 102

F

Files and Directory Structure · 135
Find Spots
  TwinSolve · 76
Flow bar · 22

I

Ice Rings · See Integrate:Ice Rings
Image window · 25
Image Window · 131
Index
  d*TREK · 63
  Overcome perceived problems · 70
  TwinSolve · 76

Index Spots · 63, See Index:d*TREK
  TwinSolve · 77
Indexing · 37
Inherited Defaults · See Defaults: Inherited
Installing CrystalClear · 15
Integration · 83

L

Log File window · 25
Logging in · 27
Login as Administrator · 141

M

Macros
  create and edit · 121
Mask Files · 54
Mercury CCD · 11
Merge Reflection Lists with d*TREK · 119
Message Window · 25

N

New Sample Defaults · See Defaults: New Sample
Next Step arrows · 25

O

Open an Existing Sample · 95

P

Predict Spots
  d*TREK · 74
  TwinSolve · 79
PROCESS · 49, 135, 151, 161, 199
Process Images · 32
Processing State · 98
Profile Windows · 131

R

R-AXIS · 11
Refine Cell
  d*TREK · 71
  TwinSolve · 78
Index

Resolution
  Set · 119
  Run mode · 21

Resolution
  Set · 119
  Run mode · 21

S
Save the Current Sample · 96
Saving Defaults · See Defaults: Saving
Scaling · 46
Scan Table · 103
  Edit · 106
  Manipulate · 105
Selecting a processing algorithm · 49
Setup · 32, 50
  Crystal1 Tab · 51
  Crystal2 Tab · 52
  Detector Tab · 53
  Main Tab · 50
  Notes Tab · 56
  X-Ray Source Tab · 55
Simulator
  Server · 112
Status Bar · 25
Step Button · 22
Steps with Substeps · 22
Stop Signs · 25

Strategy · 80
System requirements · 15

T
Task drop down list · 21
Toolbar · 22
TwinSolve · 23, 49, 76, 135, 138, 161, 199

U
Updating Defaults · See Defaults: Updating
User Preferences · 110
  Specify collection defaults · 116
  Specify directory · 111
  Specify other settings · 115
  View Settings · 110

V
View Settings · 110