INTERFACE

### History of CRYSTALS

### Understanding CRYSTALS

\*\*\* You Need to Know:

^^^ Structure database:

^^^ Lists:

^^^ Atoms:

^^^ Reflections:

^^^ Commands and Scripts

^^^ Help Files

\*\*\* Organising your data:

\*\*\* About SCRIPTS

^^^ Getting out of SCRIPTS

\*\*\* Layout of the Screen:

^^^ Main Toolbar:

^^^ Top Menu:

^^^ The Guide:

^^^ Text Window:

^^^ Summary Tabs:

^^^ Command Line:

^^^ Graphics Window:

\*\*\* Customising Crystals

\*\*\* Using The Guide

\*\*\* Using Menus

\*\*\* Inputting Data

\*\*\* Using CAMERON

### The Menus ^^^ Edit Restraints

\*\*\* Files ^^^ Add Shift Limiting Restraints

^^^ New Working Folder ^^^ Add 1-2, 1-3 Vibration Restraints

^^^ Open DSC file ^^^ Add 1-2, 1-3 Thermal Similarity Restraints

^^^ Save dsc file ^^^ Calculate Scale Factor

^^^ Save dsc file As ^^^ Recalculate Phases

^^^ Run CRYSTALS Instruction File (USE file) ^^^ PLATON Squeeze

^^^ Exit Crystals ^^^ Anomalous Modified Squeeze

\*\*\* Data \* Analyse

^^^ Open File ^^^ Agreement analysis

^^^ Open Import Guide ^^^ Fo vs Fc Graph

=== Diffractometer \*cifs\* ^^^ Difabs analysis

=== \*cif\* containing SHELX files ^^^ Wilson Plot

^^^ Data Files (Current) ^^^ Variance of Reflections

^^^ Import Shelx file (INS or RES) ^^^ Weight vs Sigma

^^^ Import HKLF4 data ^^^ Multiplicity of Observation

^^^ Import HKLF5 Data - Twinned Data ^^^ Tabbed Initial Analysis

^^^ Import Structural (CSD) \*cif\* files ^^^ Absolute Configuration

^^^ Cell, SG radiation or formula ^^^ Likely H-bonds

^^^ File Export ^^^ Rotax analysis/twins

^^^ View Reflections === Rotax

^^^ Filter reflections === Input twinned structure

^^^ Edit Scattering Factors === Remove twin laws

^^^ Edit goodies ^^^ Publication Checks

\*\*\* Diffractometer Files === Local Acta Checks

^^^ Run RC93 (Cad4 data) === Checkcif

^^^ Use RC93 output ^^^ Mogul Geometry Check

\*\*\* Solve \* Results

^^^ Tangent Recycle ^^^ Output ...

^^^ Fresh Start === Output CIF file

^^^ Known Facts === Output CIF file no esds

\*\*\* Structure === Output HTML Summary

^^^ Undo === Output Summary File

^^^ Input === Output Other tables

^^^ Edit Coordinates === Export archive files

^^^ Invert the Structure === Edit CIF goodies

^^^ Collect Atoms by Symmetry === Publication Checks

^^^ Centre Molecules === Printcif on the web

^^^ New Centre Molecules \* Graphics

^^^ Change Atom Types ^^^ Cameron Graphics

^^^ Renumber Atoms ^^^ Cameron (view existing input files)

^^^ Re-sequence Atoms ^^^ Import last Cameron output

^^^ Fix Clashes ^^^ Import last Cameron input

^^^ Allocate Residue Numbers ^^^ Mapviewer

^^^ Remove Residue Numbers \* Appearance

^^^ Allocate Part Numbers ^^^ Screen Layout

^^^ Remove Part Numbers ^^^ Atoms

^^^ Distance === Covalent

^^^ Add and Remove Bonds === Van der Waals

^^^ Add Hydrogens+Fourier === Thermal

^^^ Add Hydrogen Geometrically === Quarter size

^^^ Add Hydrogen Manually === Half size

^^^ Renumber Hydrogen === Full size

^^^ Refine Hydrogen ^^^ Model

^^^ Remove Hydrogen === Update model

^^^ Use H-files === Auto Display OFF

^^^ Create Hydrogen Restraints === Auto Display ON

^^^ Create Hydrogen Constraints ^^^ Auto scale (zoom off)

^^^ Remove Q-peaks ^^^ Set Text Font

\*\*\* Fourier ^^^ Set Input Font

^^^ Difference \* Tools

^^^ 2Fo-Fc ^^^ Preferences

^^^ Optimal === Default minimisation Function

^^^ Remove Q Peaks === Platon Executable

^^^ Set Map Ranges === SHELXT Executable

\*\*\* Refinement === External Editor

^^^ The Guide ^^^ Enable Tip of the Day

^^^ Setup Directives and Constraints ^^^ Enable TOOLS HELP

^^^ Setup and Refine ^^^ Notepad

^^^ Refinement Cycles ^^^ Delete 'bfiles'

^^^ Refine Hydrogen ^^^ Systematic Naming

^^^ Remove all Directives and Constraints ^^^ Probe Minima

^^^ Edit Directives and Constraints ^^^ Space Group Quiz

^^^ F or Fsq and Advanced Options ^^^ Who Wants to be

^^^ Choose weights ^^^ Obsolete

^^^ Rescale Weights === DELRED

^^^ Filter Reflections === Reindex

^^^ Delete all Restraints === Benchmark

=== PRIMER

=== User Guide

\* Help

### The Model Window ### The Command Line

\*\*\* Using the Model Window \*\*\* Syntax of Commands

^^^ Right Click in Background \*\*\* Types of Commands:

=== Add Hydrogen ^^^ Lists

=== Remove Fourier Peaks === Keyed LISTS

=== Geometry === Lexical LISTS

=== Mogul Geometry Check ^^^ Commands

^^^ Right Click Atom === Keyed Commands

=== Change Type of ... === Lexical Commands

=== Set Residue Number of ... ^^^ CONTINUE

=== Set Part Number of ... \*\*\* Immediate Commands

=== Set Occupancy of ... ^^^ Comments

=== Change to Uequiv ^^^ \\TITLE ..... A title to be printed .....

=== Set U[iso] ^^^ File Operations

=== Edit ... === Device Names

=== Add Hydrogens to ... === \\APPEND devicename filename

=== Split Atom ... === \\CLOSE devicename

=== Environment of ... === \\FLUSH devicename

=== Refine Mode === \\OPEN devicename filename

=== Select Fragment Containing ... === \\RELEASE devicename filename

=== Zoom to Fragment Containing ... === \\SCRIPT filename

=== Delete Fragment Containing ... === \\TYPE 'filename'

=== Centroid of Fragment Containing ... === \\USE source

=== Map Fragment containing ... onto another === \\SET FILE type

^^^ Right Click Pair === \\SET LOG state

=== Swap Labels === \\SET PRINTER state

=== Swap Coordinates === \\SPAWN 'shell command'

=== Break Bond === $ 'shell command'

=== Add Bond ^^^ Miscelaneous

=== Restrain Selection === \\BENCH nparam nref

^^^ Right Click Selection === \\COMMANDS command

=== Slant Fourier Map === ? text

=== Voids Map === \\END

=== \\FINISH

=== \\PAUSE interval

=== \\SET RATIO state

=== \\SET UEQUIV state

^^^ List Operations

=== \\SET LIST state

=== \\SET WATCH number

=== \\SET EXPORT state

^^^ System Monitoring

=== \\SET GENERATE state

=== \\SET MESSAGE state

=== \\SET MIRROR state

=== \\SET MONITOR state

=== \\SET OPENMESSAGE state

=== \\SET SRQ state

=== \\SET TIME state

^^^ Obsolete

=== \\MANUAL 'name'

=== \\HELP 'topic'

=== \\SET COMMUNICATION speed

=== \\SET TERMINAL device

=== \\SET PAGE length

=== \\SET PAUSE value

### Atomic Identifiers and Parameters ### Files and Folders

\*\*\* Atom identifiers \*\*\* Organising your data: Files and Folders

\*\*\* Atom parameter identifiers