USERGUIDE

### About CRYSTALS ### Frequently asked questions

\*\*\* Video Demonstration \*\*\* Getting Started: Organisation of files.

\*\*\* Features \*\*\* General: Who is responsible for it?

\*\*\* General: Where is the manual?

### Getting Started \*\*\* General: Is there an example to work through?

\*\*\* Organisation of data \*\*\* General: Can I prepare commands to run CRYSTALS in batch mode (like SHELX)?

\*\*\* Starting the program \*\*\* General: Is there any command line help?

\*\*\* Customising CRYSTALS to suit your screen size \*\*\* General: How can I switch the left and right CRYSTALS windows?

\*\*\* Solving structures: How do I prepare a job for SIR92 or SHELXS?

### Worked examples \*\*\* Solving structures: It failed. How do I prepare a different job?

\*\*\* Cyclo - a routine structure analysis \*\*\* Solving structures: How do I import the solution back into CRYSTALS?

^^^ Video demonstration \*\*\* CAMERON: How do I see a plot of the structure?

^^^ Discussion \*\*\* CAMERON: Can I rotate it and label the atoms?

^^^ Step one: SHELX-style data \*\*\* CAMERON: How do I delete atoms?

^^^ Step two: Initial assessment of the data \*\*\* Fourier: How do I calculate a Fourier map to find missing atoms?

^^^ Step three: Structure solution \*\*\* Refinement: What infomation does CRYSTALS need?

^^^ Step four: Commence refinement \*\*\* Refinement: Refinement instructions

^^^ Step five: Adding Hydrogen Atoms \*\*\* Refinement: Occupancies of an atom or fragment split over two sites?

^^^ Step six: More refinement & Extinction \*\*\* Refinement: How do I add restraints?

^^^ Step seven: Choose a suitable weighting scheme \*\*\* Refinement: How do you use Platon's Squeeze from CRYSTALS?

^^^ Step eight: Validation and CIF archival \*\*\* Refinement: What are parts assemblies and groups?

\*\*\* Poor Quality Data - Tetraphenylene \*\*\* Structure: How can I adjust a molecule or fragment to have ideal oordinates?

^^^ Background \*\*\* Analysis: Find the angle between a plane of atoms and a bond

^^^ Analysis and solution \*\*\* Analysis: Calculate intermolecular distances

^^^ Refinement \*\*\* Analysis: Find LIKELY H-BONDS with donors or acceptors other the O and N

^^^ But what of the e.s.d's? \*\*\* Analysis: How do I use ROTAX to test for twin laws?

\*\*\* NKET - Introduction to Command mode \*\*\* Analysis: How do I add hydrogen atoms to water molecules?

^^^ Background \*\*\* Publication: Editor wants completeness of the data at 25 degrees

\*\*\* Spacegroup Quiz \*\*\* Publication: What's the difference between \_theta\_max and \_theta\_full?

\*\*\* Publication: Diagram shows wrong enantiomer. What to do?

\*\*\* References: What References should I know about?

\*\*\* Miscellaneous: Environment variables