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The screenshot displays the TeXworks interface. The left pane shows the LaTeX source code for a document titled 'Crystallography-guide.tex'. The right pane shows the rendered PDF, 'Crystallography-guide.pdf', which includes a table of space groups and a section on solving structures.

Symbol	Space Group
$P2_1/c$	Trigonal bipyramidal
$Pbca$	Trigonal bipyramidal
$P\bar{4}$	Tetragonal

3.4 Solving the structure

There are a variety of programs for solving structures. The best choice will solve well with all of the programs on the Solve menu in WinGX and it is usually easy to use.

SIR-92 Provides a graphical interface to assign the light atoms correctly.

SHELXS-97 Two methods are available. The direct methods option is usually the one to use.

SIR-97 A more up to date version of SIR-92, tries a few more tricks and will tend to solve most small molecules.

DIRECT-2008 Choose the **PATY** sub-option: this is a heavy atom solution method, and works well if a heavy atom is present.

SIR-2004 The most powerful of the family of SIR programs, tries a very powerful set of tools but as a result can take a significant amount of time. Use this package as a last resort.

At each stage, you will probably want to take a look at the result to see whether the solution looks realistic. This can be done using the **SXGRAPH** program, which can be accessed using the icon on the WinGX toolbar.

In most cases, one or two attempts will solve the structure, with minimal adjustments to the space group or formula. When trying a number of possibilities, it is a good idea to keep a note of those tried as it can very rapidly become confusing.

4 Refinement

4.1 The process of refinement

The major part of producing a good-quality solution is refinement. This involves taking a model (from the solution), calculating the diffraction it would give and comparing that with the real diffraction. The model is then adjusted, and hopefully comes closure to giving the same intensities as were actually recorded. Refinement is an iterative process: a cycle of refinements is followed by examination of the result, adjustment and then re-refinement. This goes on until the model does not change when refined. Good overviews of the entire process of structure determination are available in the books by Clegg³ and Messa.⁴

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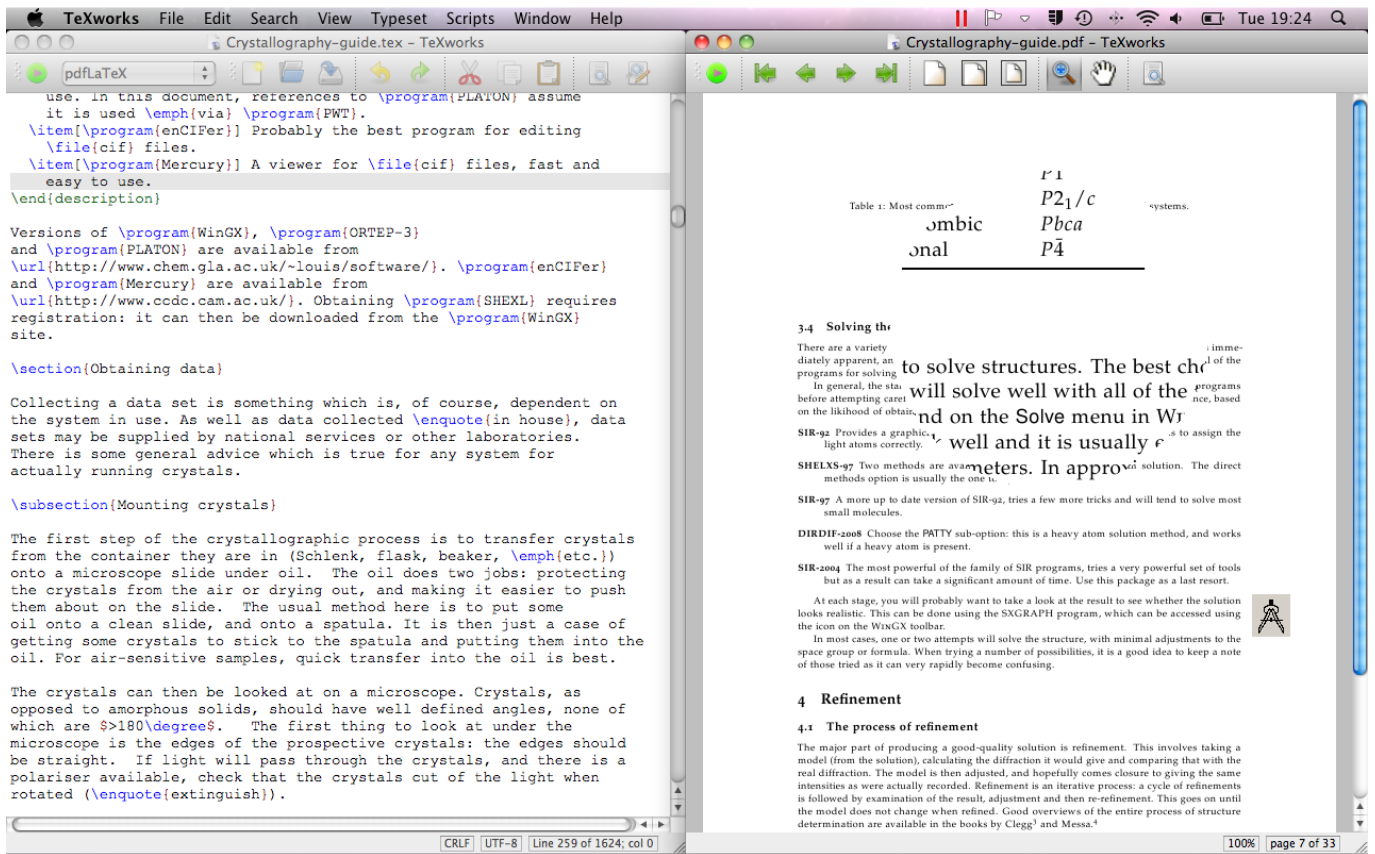
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