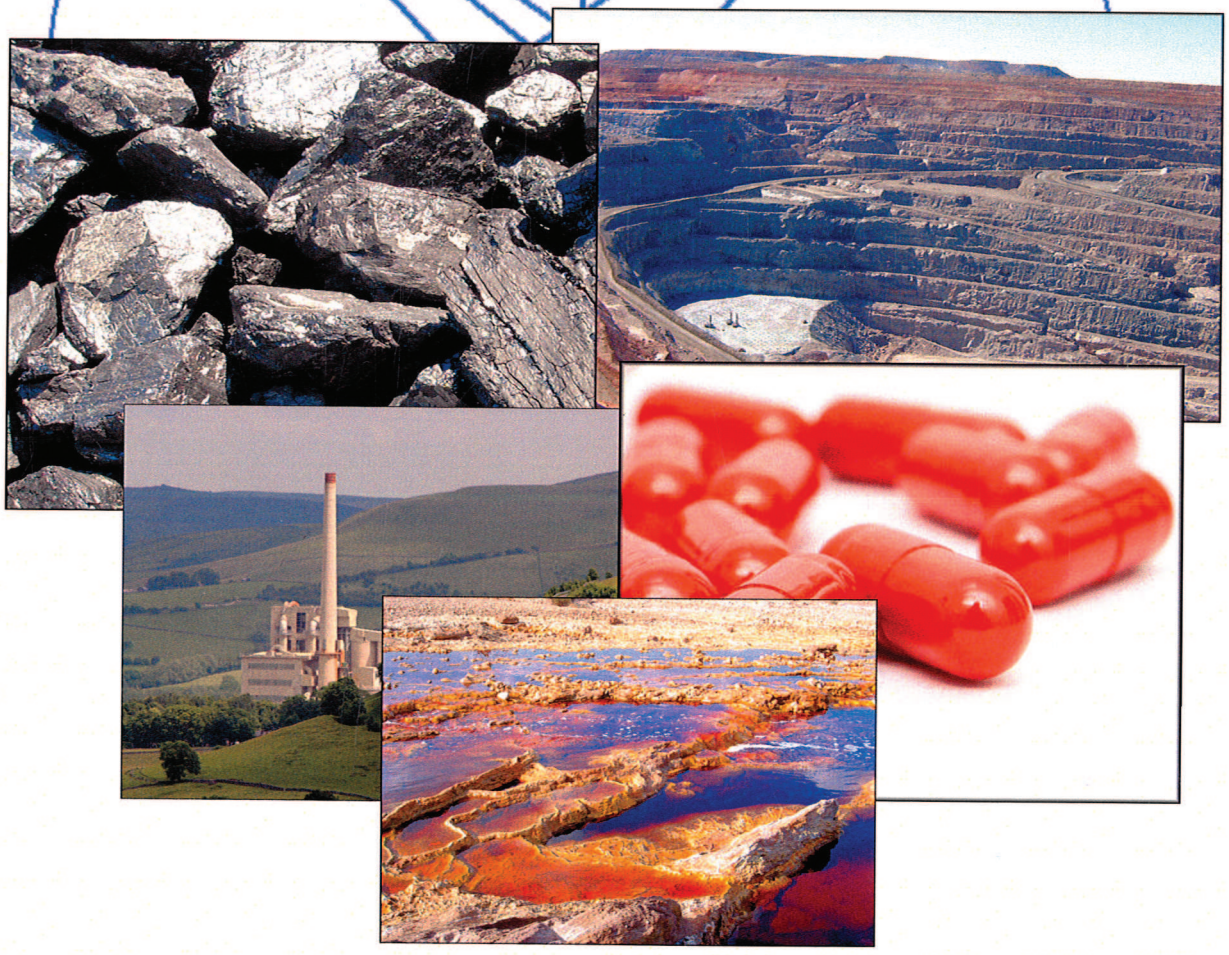
Sietronics

SIROQUANT™



QUANTITATIVE PHASE ANALYSIS SOFTWARE

www.siroquant.com

Overview of Siroquant

Siroquant is used for the quantification of phases from XRD patterns from a standard diffractometer. Siroquant is used to fit the full calculated XRD profile to the observed pattern by full-matrix least-squares refinement of the following parameters for each phase:

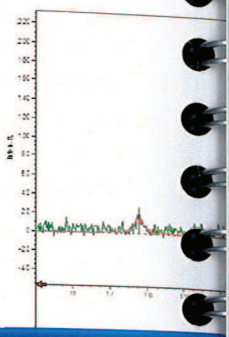
- Scale factor
- Preferred orientation
- Unit Cell Dimension
- Halfwidths (U, V, W) (with a second halfwidth available)
- The Pearson 'm' or Pseudo-Voigt lineshape parameters

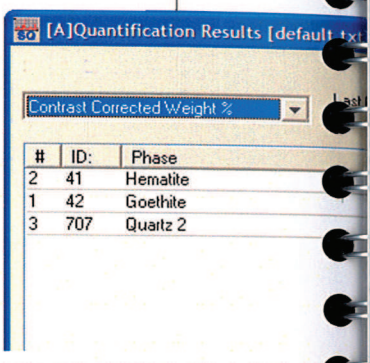
Specialist crystallographic knowledge of the minerals or compounds present in the sample is not required as the crystal structure data is resident in the Crystal Structure Databank supplied with the software. This database holds information for more than 1,700 common compounds.

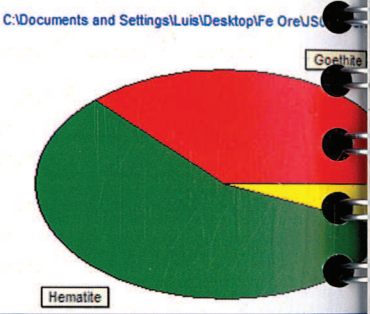
Refinement of the instrument zero and the line asymmetry parameter for the whole pattern are also supported. Point by point background subtraction is used to accurately remove the background from the pattern prior to quantification.

Corrections for the effects of particle size absorption contrast (using the Brindley correction) as well as anomalous dispersion are also supported.

Siroquant has been tested with many standard mixtures and used to quantify phases in: beach sands, Portland Cement, fly ash, coal ash, opal, clays, sandstones, slags, bauxites, china clays, zeolites, zirconia ceramics, pharmaceuticals and more!







Compatibility

Siroquant uses a standard Windows interface and can directly import most data files, including:

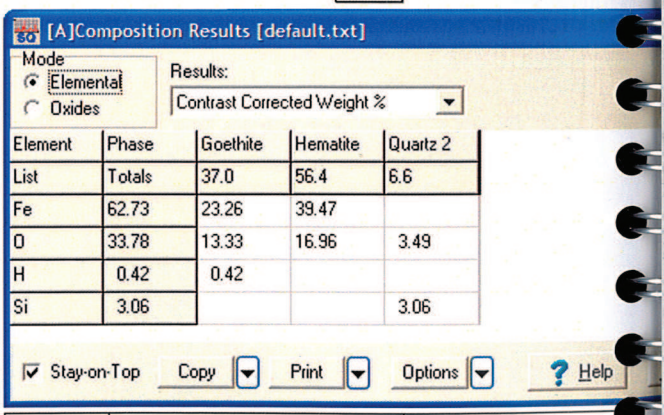
- Thermo
- InXitu
- Shimadzu
- Bruker-AXS
- PANalytical
- Rigaku
- Scintag
- Siemens
- Many other formats also supported

Easy to Use

Once the background has been corrected, an automatic prescaling gives a good ballpark first profile fit in a matter of seconds – this is then the starting point for further refinement if required.

Graphical functions include a zoom function for a detailed study of the fitted pattern and (hkl) bars for phase identification. The user can use graphical display of residuals using the chi-squared function and mean parameter shift per phase over the refinement stages.

Output of quantification is available as a pie chart or numerical listing and can be copied to the windows clipboard. There is also the facility for colour printer publication mode graphics output.



	Partial XRF analysis	Siroquant Back Calc
Fe	62	63
H2O	4	5
SiO2	7	6

Comparison of Siroquant results with XRF an

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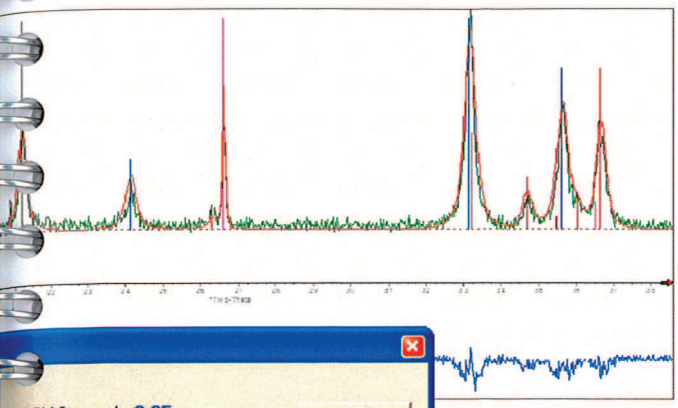
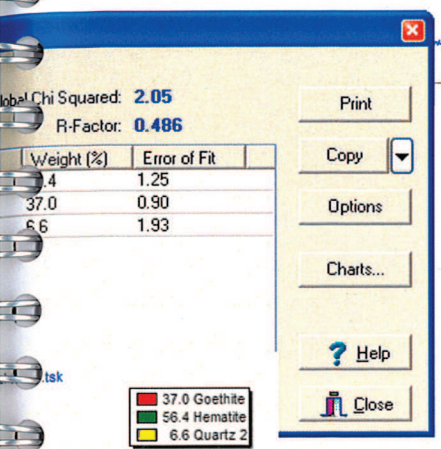




Features

Amorphous Content may alter the Rietveld quantitative results. The program can be used to correct for the overall amorphous content by using a spike phase. Individual phase amorphicities may also be included if known from chemical analysis.

Absorption Contrast corrections are very important when the phases have different X-ray absorptive power and within Siroquant these corrections are calculated according to Brindley.

Each phase has a refinable Preferred Orientation parameter available using the March function. The user specifies the plane on which the orientation is occurring and a single orientation parameter is refined by the program to fit the measured data.

Analysis of Clays:

Normally, crystal structure data is needed to quantify a mineral with the Rietveld method. Minerals with unknown or imperfectly known crystal structures (e.g. clays) can still be quantified with Siroquant. To do this an 'observed (hkl) file' is used, instead of the normal calculated file, to give a standard Rietveld profile for the mineral. Observed (hkl) files for use with Siroquant have been prepared for clays including montmorillonite, kaolin, illite, halloysite and palygorskite.

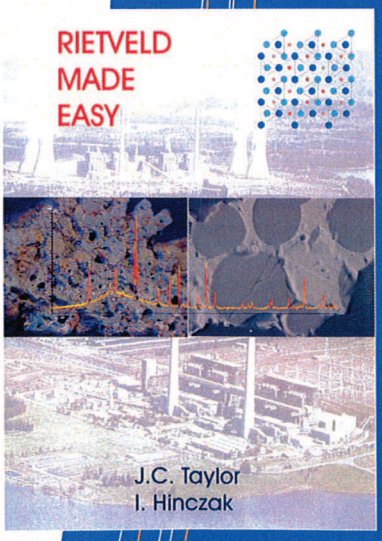
Additional Features

- Determination of crystallite size
- Determination of chemistry via back calculation
- Determination of cell parameters
- Any number of phases present in each task

Rietveld Made Easy

This book is designed as a practical guide to the fundamentals of crystallography as applied to Rietveld analysis and is an essential companion to the User Guide supplied with Siroquant. The introduction to the book is available from the Sietronics Website.

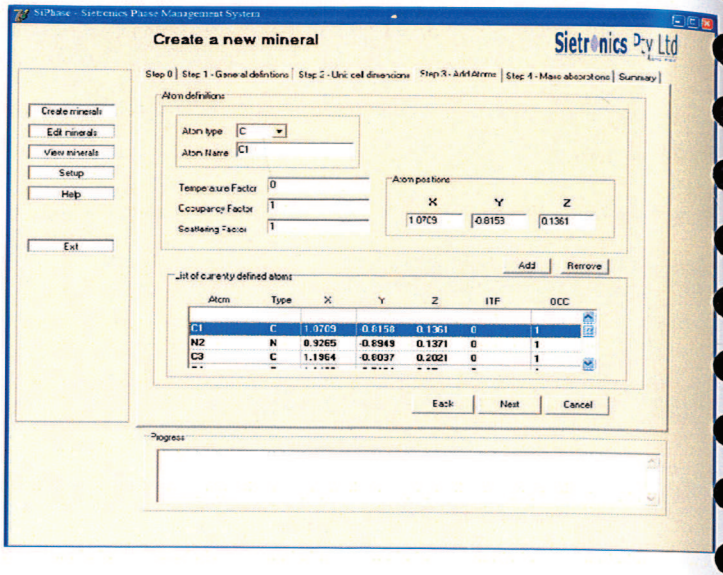
Copies of the book can be ordered directly from Sietronics.



SiPhase

New software that allows phases to be easily entered into the Siroquant phase database.

- Easy to use
- Phases can be read directly from CIF files, or can be done manually
- Compatible with Siroquant V3
- No crystallographic knowledge required



Siroquant Users Forum

Sietronics is pleased to announce the creation of the Siroquant User Forum. To sign up to the forum go to www.siroquant.com/forum to:

- Find out how to get started
- Get answers to common problems
- Learn new ways of doing things
- Get advice on difficult applications

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