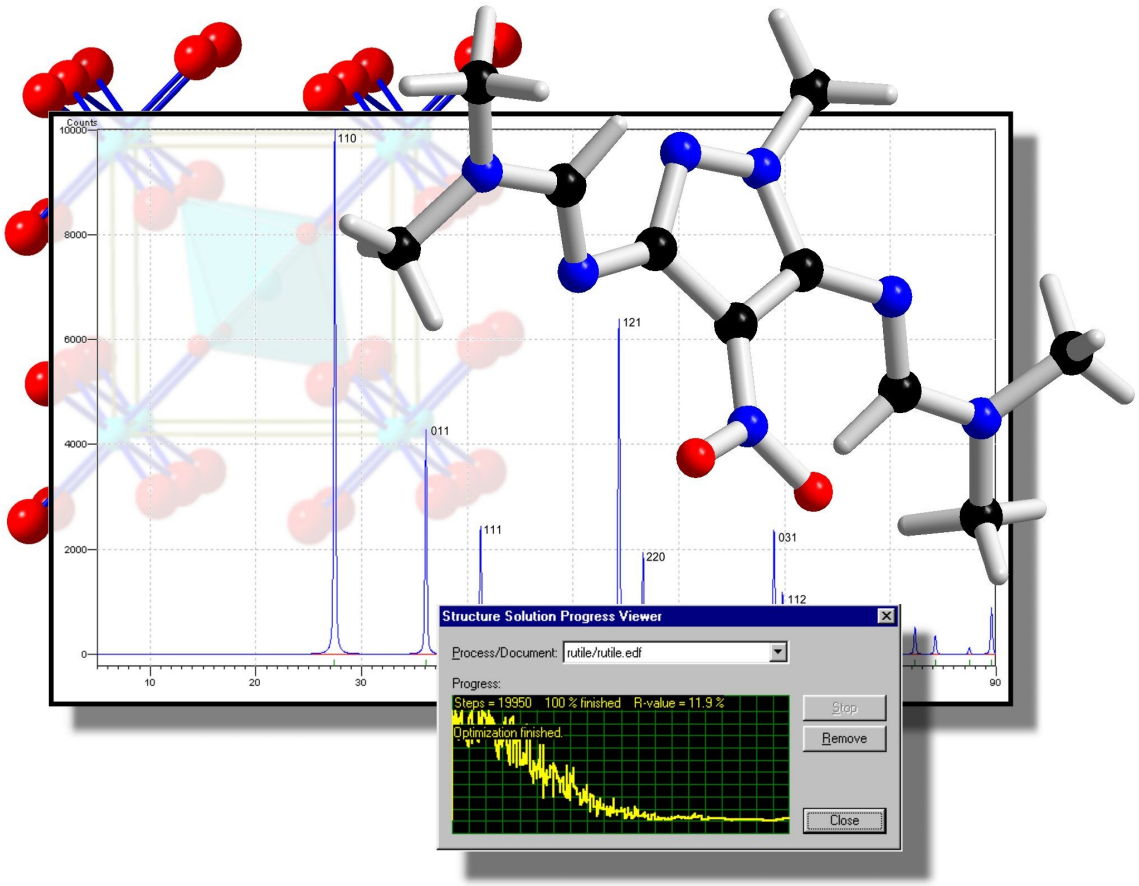
ENDEAVOUR

Structure Solution from Powder Diffraction

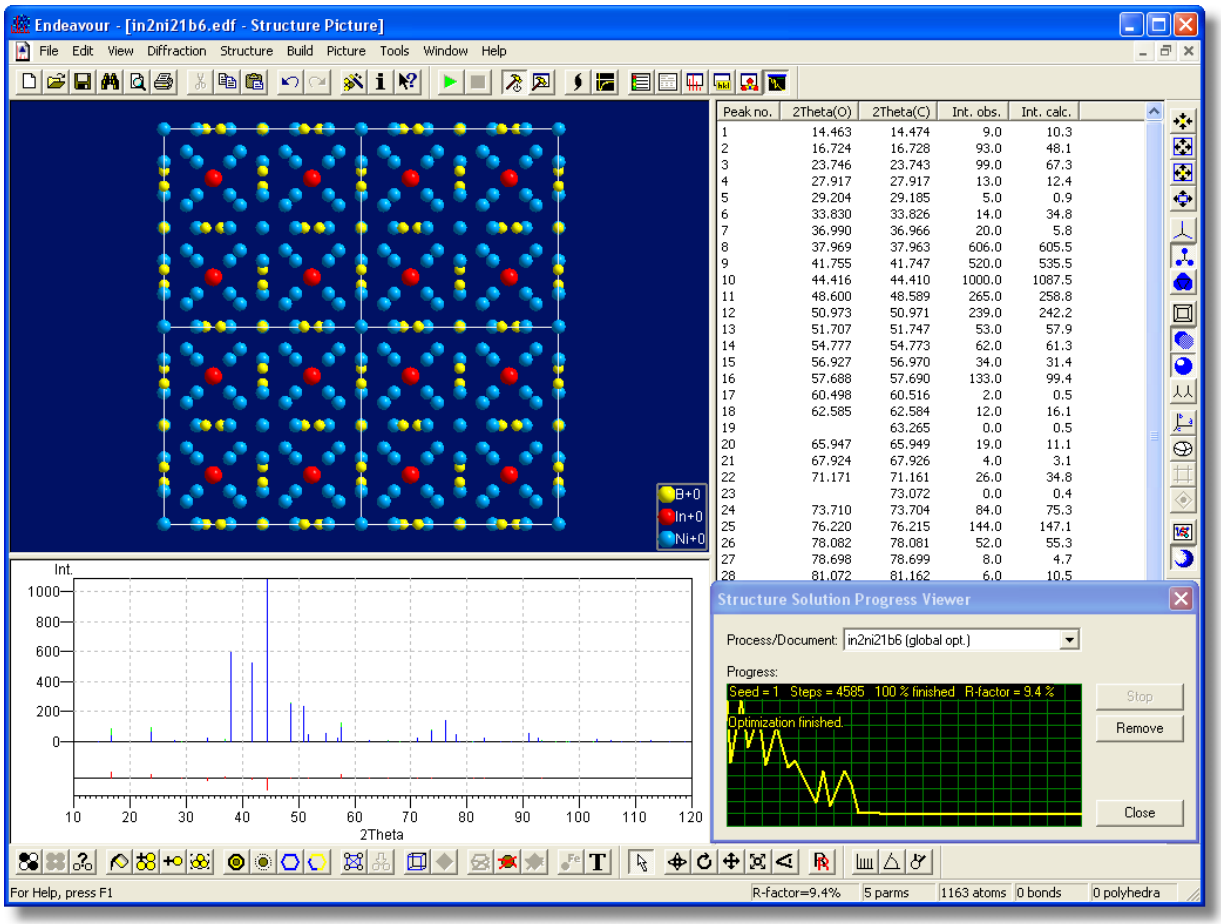


See what's behind it !

CRYSTAL IMPACT

ENDEAVOUR is a powerful software for structure solution from powder diffraction data, closing the remaining gap between indexing and Rietveld refinement. The combination of its innovative concept and its elaborate user interface makes solution of small to medium sized crystal structures from powder an almost routine process, both for organic and for inorganic materials.
The structure solution is performed using a special variant of the "direct-space" approach, namely a combined global optimization of the difference between calculated and observed diffraction pattern and of the potential energy of the system.
All you need are the unit cell parameters, the composition and of course the powder diffraction data (integrated intensities at Bragg angles 2theta) or structure factors |F(hkl)| obtained from Le Bail or Pawley fit or even single crystal diffraction data.

Even unexperienced users can prepare and perform the structure solution calculation in a few steps, guided by the integrated "wizard".



Features

- Structure solution from X-ray laboratory, synchroton, neutron or electron diffraction data
- Input required: cell parameters, peak list (2theta vs. intensity; no profile step-scan data), contents of the unit cell (composition or molecule structure plus number of formula units)
- "Wizard" for the easy preparation of the input data
- Viewing of the intermediate steps of the structure solution process: structure picture, progress (%finished), R-Factor, etc.
- Support for molecular structures (incl. rotatable bonds) as well as for atomic structures with single atoms on special positions
- Hofmann potential for solving/predicting molecular structures
- Automatic variation of special positions for single atoms during structure solution calculations in space groups higher than P1
- Structure solution/prediction either by energy minimization or from diffraction data alone is possible
- Symmetry Finder with automatic transformation
- Elaborate crystal structure visualization facilities similar to DIAMOND
- Online update option (automatic or manual)

System Requirements

- Microsoft Windows 95, 98, ME, NT4, 2000 or XP
- Pentium II / compatible processor (or higher)
- 32 MB of RAM (64 MB recommended)
- Graphics resolution of 800 x 600 pixels with 256 colors (1024 x 768 pixels or higher with 32,768 or more recommended)
- 20 MB of free disc space
- **Supported diffraction data file formats**: Stoe (*.pks), Philips/PANalytical (*.idf, .udi), |F(hkl)| list (*.hkl), peak list (2 columns: 2theta/d intensity; *.dif)

Prices*

	non-profit org.	profit org.
Single licence	749 €	1,498 €
Site licence**	1,498 €	2,996 €
Campus licence***	2,996 €	5,992 €

* Prices do not include taxes which may be due.
** Unlimited number of installations within one institute/dept.
*** Unlimited number of installations within one university/company

CRYSTAL IMPACT

CRYSTAL IMPACT GbR
Postfach 12 51
D-53002 Bonn
Germany

Tel: +49 (228) 981 36 43
Fax: +49 (228) 981 36 44
E-mail: info@crystalimpact.com
http://www.crystalimpact.com