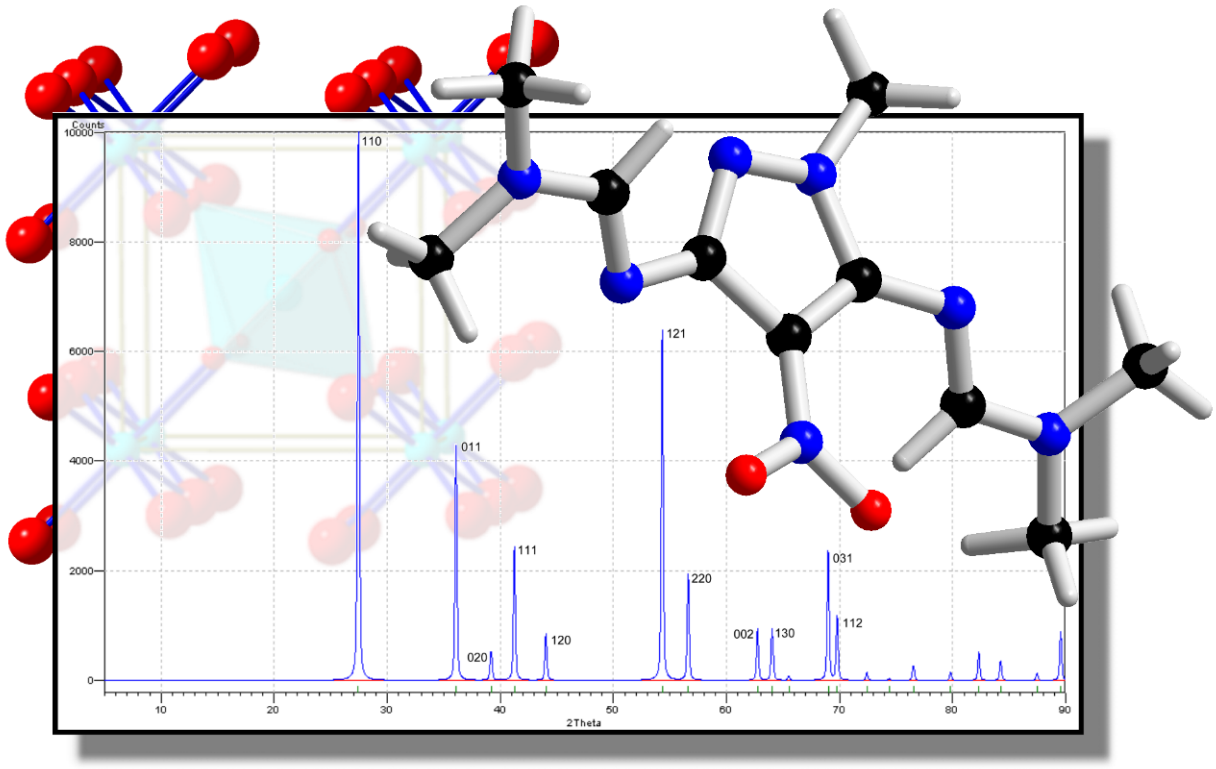
ENDEAVOUR

Structure Solution from Powder Diffraction

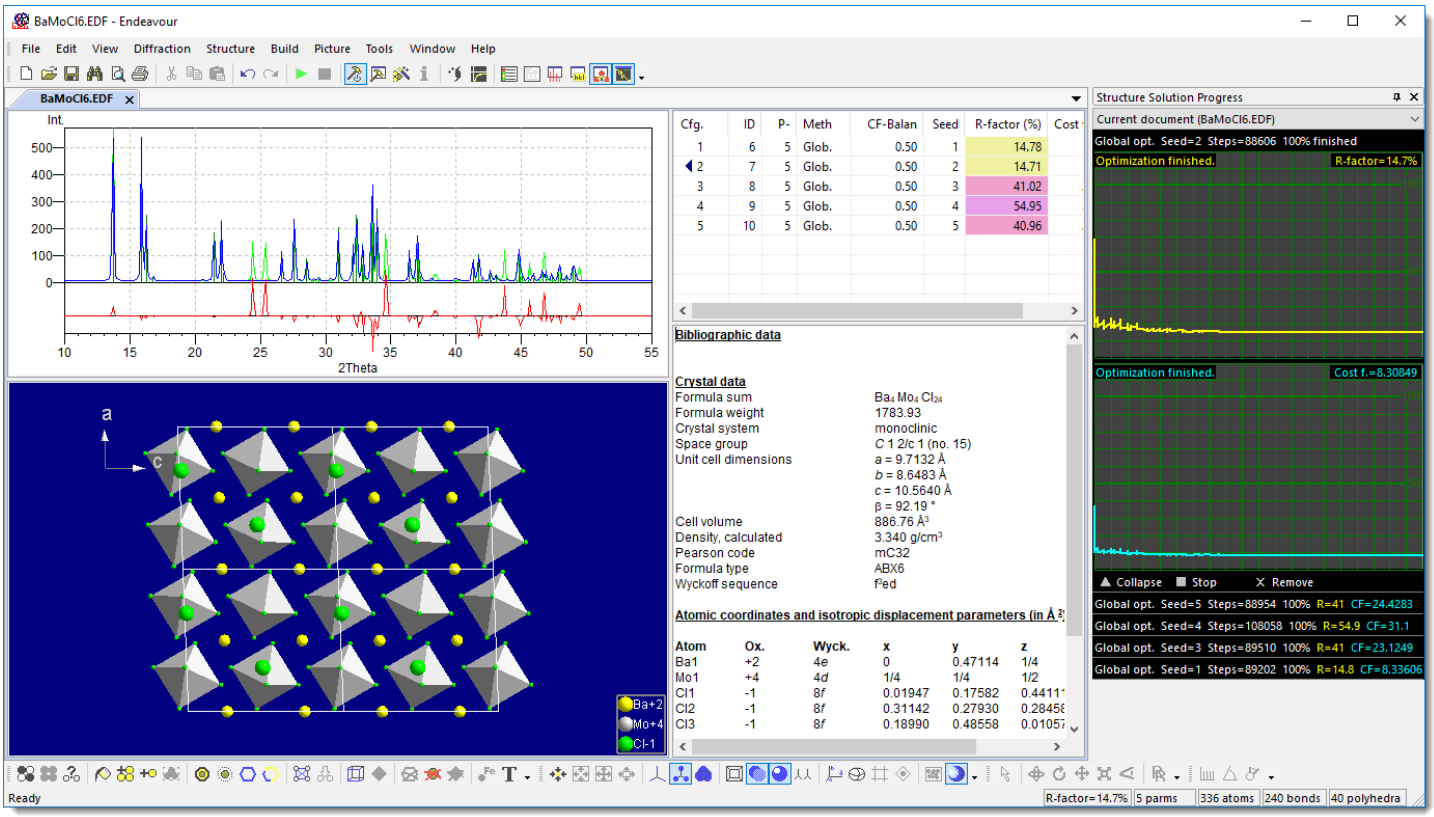


Combines potential energy and R-factor optimization in a unique direct-space approach

CRYSTAL IMPACT

ENDEAVOUR is a powerful software for crystal structure solution, both from powder as well as single crystal diffraction data. Based on more than twenty years of experience, the software can solve many small to medium sized structures more or less on its own. The innovative concept combined with the elaborate user interface makes solution of crystal structures an almost routine process, especially for inorganic but also for many organic compounds.
Even unexperienced users can prepare and perform the structure solution calculation in a few steps:

Simply follow the integrated "wizard" to enter the required data (unit cell parameters, chemical composition, diffraction data), and let Endeavour do the rest.
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 data and of the potential energy of the system. Due to the additional usage of the potential energy, the method is much less sensitive to low-quality diffraction data than e.g. direct methods.



Feature

- Structure solution from X-ray laboratory, synchrotron, neutron or electron diffraction data
- Required input: unit cell parameters, chemical composition / molecule structure, diffraction data
- Powder diffraction data (integrated intensities at Bragg angles 2theta) or single crystal diffraction data (I(hkl), |F(hkl)| or F^2(hkl)) can be used
- "Wizard" for the easy preparation of the input data
- Automatic adjustment of calculation parameters
- Automatic space group determination from resulting structure
- Viewing of the intermediate steps of the structure solution process: structure picture, progress (%finished), R-Factor, etc.
- Support for structures with single atoms on special positions as well as for molecular structures (incl. rotatable bonds)
- 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

System requirements

- PC with Windows XP, Vista, Windows 7, 8, 10 or 11
- Microsoft Internet Explorer 5.01 or higher
- 64 MB of RAM
- 100 MB of free disk space
- Graphics resolution of 1024 x 768 with 32,768 colors (”High Color”)
- **Supported diffraction data file formats**: Stoe (*.pks), Philips/PANalytical (*.idf, .udi), I(hkl), F^2(hkl) or |F(hkl)| list (*.hkl), peak list (2 columns: 2theta/d intensity; *.dif)

Prices

	non-profit org.	profit org.
Semiannual license (6 months)	149.50 €	299 €
Annual license (1 year)	299 €	598 €
Single license (permanent)	599 €	1,198 €
Site licence (permanent)	1,198 €	2,396 €
Campus licence (permanent)	2,396 €	4,792 €

* Prices do not include taxes which may be due.

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