

## JANA2006, version 03/05/2011

### New version of Jana2006 for Windows is available in [jana.fzu.cz](http://jana.fzu.cz)

Dear users of Jana software,

We have pleasure to announce the new maintenance release of Jana2006 for Windows.

#### ***What's new:***

**(Tools-Transformations)** New possibility to change an enantiomorph.

**(Tools-Special tools)** Improved procedures for simulation of powder and single crystal data

**(Refine)** New option for keeping rigid geometry without introducing "molecules"

**(Powders)** New correction functions for asymmetry of TOF powder data. • LPG correction for Guinier camera.

**(File-Reflection file)** New tool for making a manual culling has been developed. Averaging results and statistics and/or  $F(\text{obs})-F(\text{calc})$  differences from the refinement are used to localize and eliminate "bad" reflections.

**(File-Import model)** New possibility to use Amplimodes, in the form as supplied by Bilbao Crystallographic Centre. • New possibility to import structure model from SHELX or CIF

**(File-Structure-New)** New possibility to import data and structure from Protein Data Bank.

**(Fourier)** Improved procedure for charge integration

**(File-CIF Utilities)** For CIF output Jana provides new specific CIF keywords for description of more complicated modulated or twinned structures.

**(Drawing)** When launching a drawing program (Diamond, Mercury etc.) the user can choose two modes: Jana either waits inactively for finishing or repetition of plotting or it is immediately active alongside with the plotting program. The drawing tool also offers pre-selection of atoms and Fourier peaks and (for magnetic structures) Bohr magneton to Å relation.

#### ***A lot of another small improvements and bug fixes***

UNIX version: still under development

Cookbook on Jana2006 cumulates workshop examples. The latest version [jana.fzu.cz/workshops/cookbook.zip](http://jana.fzu.cz/workshops/cookbook.zip)

**We wish you a lot of successful refinements with Jana2006!**

Best Regards,

*Vaclav Petricek*

*Michal Dusek*

*Lukas Palatinus*