JANA2006, version 23/10/2008

This announcement is being sent to everyone who has registered as a user of Jana software.

Maintenance release of Jana2006 for Windows is available in www- xray.fzu.cz/jana

Dear users,

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

Development

- Powder option – fundamental approach: The program now allows correcting for variable slit divergence. Moreover a diffraction technique (Debye-Scherrer, Bragg-Brentano, etc) can be specified during data import. This information is later used to avoid improper combinations of powder parameters.

- EditM50: (1) The check for consistency of cell parameters and modulation vectors with the symmetry is now made only once when the dialog is closed. Moreover the program now offers modification of cell parameters to achieve consistency with the symmetry. (2) New possibility to select space and superspace group symbols from the list.

- Space group test: new possibility to see list of reflections violating extinction rules and reports from merging reflections for each offered symmetry.

- Transformations: added list of predefined transformation matrices, for instance from R to P elementary cell.

- Dist: Dihedral angles between planes are shown as a function of t (for modulated structures).

- Grapht: added possibility to call program DPlot (www.dplot.com)

- Interface: external programs have been moved from Preferences to Tools->Programs

- UNIX version is still under development.

. . . . and many other small improvements

Bugs

- Transformations: (1) Non-integer transformation matrices did not transform correctly diffraction indices. (2) Transformation to a subgroup did not work properly for crenel functions with orthogonalization. (3) False messages about unrealistic centering vectors.

- Absorption correction: cylindrical absorption correction for $Mi*r > 8$ did not work correctly

- Multiphases: problems when more than one modulated phases was present.
- Refine: false warnings about improper fixing of x4 origin.
- Dist: wrong bond valences were calculated for atoms in special positions (for modulated structures)
- Powders: Profile viewer did not work correctly for profiles simulated by Jana
- CIF: Fo-Fc list was not created.
- Data repository: reimport did not work correctly for cases when original data were transformed by the space group wizard.

. . . . and many small bug fixes

Versions terminology

STABLE versions of Jana2006 contain cumulated and tested corrections and improvements. This announcement is about stable version.

LAST versions of Jana2006 contain the latest development.

BETA versions will be testing version of Jana2012. Not yet available.

FINAL versions are closed, this is Jana2000.

The Download table in Jana web page displays the version string, for instance 23/10/2008, which is also visible in Tools -> About Jana2006.

Roadmap:
- Finishing manual
- Porting Jana2006 to Unix
- Finishing magnetic structures
- Polishing all features
- Starting development of beta version Jana2012 with completely new interface

We wish you a lot of successful refinements with Jana2006.

Best Regards,

Vaclav Petricek
Michal Dusek
Lukas Palatinus