JANA2006, version 23/10/2010
New version of Jana2006 for Windows is available in jana.fzu.cz

Dear users of Jana software,

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

What's new:

(EditM50) New routine for checking of consistency between cell centering and the symmetry operations.

(Symmetry wizard) Removed bug concerning testing of X centering for hexagonal symmetry. • Removed bug concerning search for supercell space group from superspace symmetry of commensurate structures, in cases when the supercell is described by a general matrix.

(Tranformations) Removed bug concerning transformation matrices with determinant different from one.

(Contour) Removed bug concerning calculation of p.d.f. and j.p.d.f. error maps. • Removed bug causing incorrect angles between internal vectors for 5d and 6d structures.

(Refine) Removed bug causing that calculation of structure factors for modulated structure failed if the first atom had zero occupancy. • Removed bug concerning refinement of modulated rigid bodies.

(Multiphases) Improved import of a new phase. • Improved procedure for setting automatic refinement keys for modulated multiphases.

(Powders) For TOF data an incident spectral file is now read and used in the refinement.

(Tools-Graphics) New indexing and refinement tool

(Input wizard) New option to write M91 in e format. • For Oxford Diffraction input Jana2006 can read experimental CIF file instead of SUM file. The advantage of CIF over SUM is that CIF contains additional information about the experiment.

(Dist, Atom Edit) Typical distances taken from IT vol. C are now distributed with new versions of Jana2006. They are used to limit distance calculations and create molecular motifs. In the case that for given pair of atoms values are not available the program uses atomic radii instead. Moreover a user can define own values. • Dist now take into the account s.u.'s of cell parameters. • Improved procedure for searching hydrogen bonds

Small improvements and bug repairs

UNIX version: still under development
Cookbook on Jana2006 cumulates workshop examples. The latest version jana.fzu.cz/workshops/cookbook.zip

We wish you a lot of successful refinements with Jana2006!

Best Regards,

Vaclav Petricek
Michal Dusek
Lukas Palatinus