Towards the Routine Application of Computing System Jana2000

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The program Jana2000 [1] was originally written as a special refinement tool for modulated structures. During almost 20 years of development it integrated many crystallographic methods that gave the program exceptional flexibility. On the other hand, it has been always difficult keeping all the possibilities accessible not only for specialists, but for everybody interested in solution of a modulated structure. With progress in the experimental methods the number of modulated structures grows amazingly. Many of them can be solved relatively easily using just the basic knowledge about aperiodic crystals.

We anticipate this trend by creating set of wizards for guiding the user to solution of simple structures, keeping - of course - all possibilities opened to complicated cases. This development is far from completion but important steps have been already done. First of all - unified tools are available for standard and modulated structures and also for powder and single crystal data that allow solving the basic and modulated structure using the same program. The phase problem (in three dimensions) can be resolved by rendering the data to SIR or EXPO and reading back the results. Automatic symmetry determination is possible for space as well as super space groups. Adding of hydrogen atoms (and generally defining geometry constraints for standard and modulated structures) has been automated to the extent usual in routine crystallography. In the lecture we shall present the outlined methods and envisaged features of Jana2005.

[1] http://www-xray.fzu.cz/jana/Jana2000/jana.html
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