s9.m29.o1 **Avoiding and Detecting Errors in X-ray Crystal Structures of Small Molecules**. Martin Lutz and Anthony L. Spek, *Dept. Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands. E-mail: m.lutz@chem.uu.nl*

Keywords: Optimization; Validation; Structure quality

With the introduction of area detectors for the X-ray diffraction experiment, the data collection time has decreased dramatically. The manufacturers provide elaborate software packages which make the experiments accessible also for the inexperienced scientist. Consequently more and more chemists without a crystallographic education are determining crystal structures and publish the results. This has led to an increased amount of published structures during the last years. Unfortunately some of these structures are suboptimally determined or even substantially wrong.

From the experience in a service crystallography laboratory useful advise for an optimal result will be presented:

- Crystal growth, selection and handling are the first crucial steps in the determination of a crystal structure.
- Optimal experimental conditions (temperature, wavelength, scan mode, etc.) to improve the quality of the results will be given.
- Pitfalls in the indexing procedure and space group determination will be explained. Refinement errors and possible solutions to avoid them will be mentioned.
- Useful software tools for the validation of crystal structures will be presented [1]. Some frequently encountered errors in the literature will be explained.

[1] A.L. Spek (2003). *J. Appl. Cryst.* **36**, 7-13.

s9.m29.o2 **SYSTER and ISOQUEST: How good and unique are your data and structure?** R. de Gelder and J.M.M. Smits, *NSRIM Institute, Radboud University Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands. E-mail: rdg@sci.kun.nl*

Keywords: Data Analysis; Structure Comparison; Pattern Matching

Once a crystal structure has been solved the question is always a) how well the structural model fits the diffraction data and b) whether the structure is new compared to the collection of structures already recorded in literature and databases. The SYSTER and ISOQUEST programs [1] were developed to answer these two questions in a convenient and rapid way. SYSTER gives the user the opportunity to analyse the match between originally observed and calculated diffraction data in the form of one, two or three-dimensional representations of reciprocal space. Various scaling regimes can be applied to the data to analyse the specific distribution of errors and the role of weighting schemes. The effect of subsequent refinement and/or data correction steps can be visualized. In this way the user might trace systematic errors related to the measurement, data reduction step, absorption correction or model refinement that cannot be derived from global agreement factors alone. The ISOQUEST program compares your structural model with all crystal structures currently present in the CSD (Cambridge Structural Database [2]) for which 3D-coordinates are available. The usual procedure for checking the uniqueness of a structure or for finding related chemistry in the CSD is defining a search in the Conquest program of the Cambridge Crystallographic Data Centre (CCDC). Such a search can be based on a chemical fragment, the unit cell, a space group, the chemical composition etc. For several reasons it is quite easy to miss closely related structures and chemistry. This is not necessarily a shortcoming of the CCDC software or the user's experience but is a result of chemical variety that cannot be anticipated easily: atoms, substituents, ions, complete molecules and bonds might be replaced by other types without a significant change in crystal packing. A unit cell search often gives too many hits and using the space group is risky when you have phase transitions or symmetry breaking, as a result of a change in temperature, small chemical modifications or polymorphism. Using the ISOQUEST program, which is based on an extension of pattern matching techniques developed by us earlier [3], complete and often surprising lists of identical or related structures can be found in the CSD, in less than half a minute on a modern PC. Similar structures can be further explored with ISOBASE, a database which contains all isostructurality relations in the CSD. This prevents a scientist from unintentionally publishing a re-determination or from overlooking relevant structures and literature. For both the SYSTER and ISOQUEST programs some theoretical background will be given and illustrative examples will be shown, demonstrating the usefulness of the two programs.

[1] Executables will be available at: http://www.crystallography.nl
[2] F. H. Allen (2002). *Acta Cryst*. **B58**, 380-388.
[3] R. de Gelder, R. Wehrens and J.A. Hageman (2001). *J. Comp. Chem*. **22**, 273-289.