Fully Automated Small Molecule Structure Determination; A Crystallographic Dark Laboratory. Michael Hursthouse*, Mark Light and Yang Li, *School of Chemistry, University of Southampton, Southampton, Hampshire, SO17 1BJ, UK*. E-mail: light@soton.ac.uk

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Ever decreasing data collection times and an explosion in demand present us with the situation where an automated single crystal structure determination process is not only advantageous but essential. Recent developments in software, instrumentation and robotics have made it possible to fully automate structure determination, from mounted crystal to completed crystal structure. In Southampton we have developed a system that takes pre-mounted samples, loads them onto the diffractometer, assesses their diffraction quality, determines the unit cell, calculates and performs the data collection, carries out data reduction, and finally solves and refines the structure. A completely integrated approach means there are no bottlenecks at any one point in the system and control and data flow easily from one stage to the next. Where appropriate we have used existing methods and programs but in general a new ground up approach has been opted for. This has involved significant divergence from the protein world, resulting in a system aimed very much at the chemical crystallography lab. The data collection procedures are built around and adapted from the Collect suite of programs[1] using PYTHON. The structure solution and refinement program, SYSTEM-Y, is written in FORTRAN and based on the SHELX [2] suite of programs. It is designed in a way that emulates the decision making processes of a human crystallographer. Throughout the development of the system the emphasis has continually shifted as potential pitfalls were uncovered and then solved. These included crystal mounting, scan parameter calculation, collision security, space-group determination, atom typing and validation of structure. Our approaches to these pitfalls will be discussed.

[1] "Collect" data collection software, Nonius B.V., 1999.

[2] SHELX97, Programs for Crystal Structure Analysis (Release 97-2). G. M. Sheldrick, Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.