A Fully Automated Diffraction System for the Small Molecule Laboratory, Mark Light,* Michael Hursthouse and Yang Li, *School of Chemistry, University of Southampton, Southampton, Hampshire, SO17 1BJ, UK*. E-mail: light@soton.ac.uk

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The advent of CCD detectors and bright lab X-ray sources has accelerated the diffraction experiment to a point where a small molecule data set can be collected in as little as a few minutes, or more routinely in a few hours. Thus, to fully utilise the instruments capability some level of automation is essential. In our lab in Southampton we have taken the approach of automating the entire process, from mounted crystal to refined structure. A pre-mounted sample from a rack of 24 is loaded onto a Kappa CCD diffractometer by a BruNo sample changing robot. Prescans are performed to asses the crystal diffraction quality and, if favourable, a unit cell is determined. Data collection is carried out using a calculated strategy based on the diffracting power of the crystal and the unit cell dimensions. Data reduction takes place as a parallel process and finally the structure is solved and refined. Key points in the development of the system included the automation of the diffraction experiment, intelligent decision making, integration of the diffractometer and sample changing robot, automation of structure solution and refinement, and development of a controlling GUI. The automation software is written in PYTHON and utilises the documented diffractometer control and data collection software modules of COLLECT [1]. This made possible the full integration of the system flow between the robot and diffractometer and substitution of all required user inputs. A user interface, X-Tray, has been written to initialise the experiment and set various global parameters. The structure solution and refinement program, SYSTEM-Y, is written in FORTRAN and is based on the SHELX [2] suite of programs.

[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.