Automatic Element Assignment and Model Completion for Small-Molecule Structures

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From reflection file to fully assigned and validated structure – from dream to reality. We will present new software which needs nothing more than the reflection file, the unit cell dimensions and some information about the crystal symmetry. From this starting point, a variety of tools are employed to solve the structure and then correctly assign the atom types, including hydrogen positions. In most routine cases, a correctly assigned and finished structure, complete with IUCr cif-check report and ready-to-submit ".cif" files will result without the need for intervention.

The crystallographic core of this software is provided by G. M. Sheldrick. XS, XD and XL have earned the trust of many crystallographers during decades of wide-spread use in the community. These new tools build on this proven crystallographic basis and are designed to work with the Bruker axs "Apex" software suite. We will present in detail their effectiveness, limitations and detailed roles in the process of fully automatic structure solution and refinement. Issues arising from twinning and disorder as well as incomplete or missing formula and their impact on the system will be discussed.

Keywords: small molecules, structure determination, automated software