s9.m30.o4 **SIR2002: its heir SIR2004 and IL MILIONE.**
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SIR2002 is a well established program for the ab initio crystal structure solution of small-, medium - and macro-molecules ([1]Burla *et al.* 2003). It does not need prior information but requires atomic resolution for the experimental data. The heir of **SIR2002**, the package **SIR2004**, is under beta-testing. It shows several advantages :

1) the sequential procedure of SIR2002 (all the trials provided by the tangent procedure are sequentially refined in direct space) is replaced by a faster procedure using early figures of merit just after the tangent step. This eliminates non promising trials and makes the procedure much faster.
2) the phasing process has been powered, and allows to solve protein structures even if data have quasi-atomic resolution (1.4 A) ([2] Burla *et al.* 2003).

SIR2004 has been implemented into the package **IL MILIONE**, a set of programs designed for global phasing.

It is able :

1) to combine direct methods with SIR-MIR, SIRAS-MIRAS, SAD-MAD techniques (i.e., substructure determination, structure factor phasing, solvent flattening).
2) to solve and refine crystal structures from powder data.

[1] M.C. Burla, M. Camalli, B. Carrozzini, G.L. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna. J. Appl. Cryst. (2003), **36**, 1103.
[2] M.C. Burla, B. Carrozzini, R. Caliandro, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori. Acta Cryst. (2003), A**59**, 560-568.

s9.m30.o5 **The System-S Approach to Automated Structure Determination: Problems and Solutions**.
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A completely automatic crystal structure determination of an organic or metal-organic compound, i.e. from space group determination to a validated and publishable result, can be trivial when based on good low temperature data and correct prior knowledge of the chemical composition. On a modern workstation (e.g. a 3GHz XEON/Linux PC) the whole process may take in the order of seconds rather than minutes with the SYSTEM-S implementation in PLATON[1]. In practice, the situation is often more complicated. More than one a-priori space group may be applicable given the observed systematic extinctions. The underlying (pseudo)-merohedral twinning may have been not detected at the start of the analysis, i.e. no split reflections or reflections not fitting in the lattice were seen on the diffraction images. The structure may not solve with the method of choice or only in a lower symmetry space group. The actual chemical composition often deviates for various reasons significantly from the assumed one. Parts of the structure may be disordered requiring expert human interaction to create a disorder model. Solvent accessible voids may contain disordered solvents, often with unknown identity or mixtures. The correct assignment of element types may be problematic (e.g. S and P, when both are present in the structure). The positive detection of hydrogen atoms, essential for the chemistry involved, may be difficult. Various tools, many of which are available in PLATON, can be used to address those complications. Among those are VALID[2] for the val;idation of the results of the structure determination, ADDSYM for the detection of missed higher symmetry in a refined structure, the SQUEEZE procedure for handling the disordered solvent problem and TwinRotMat for the detection and handling of various twinning issues. The latter routine will, based on large positive F(obs) – F(calc) differences, determine the effective twin matrix and produce the proper 'HKLF 5' style reflection file to implement the subsequent twin refinement with SHELXL97.

[1] http://www.cryst.chem.uu.nl:platon
[2] A.L.Spek, *J.Appl. Cryst*. **36** (2003) 7-13.