Automatic Structure Determination. Is it Just a Dream? D.J.Watkin & R.I.Cooper *Chemical Crystallography Laboratory, 9 Parks Rd, OXFORD, OX1 3PD, UK*

Keywords: Validation; Automation; Analysis

"Methods have been developed by Ford, Hodgson, Rollett & Stonebridge (unpublished) for automatic solution of crystal structures".[1]

Some of this 30 year-old optimism has been justified by subsequent events. SIR92 and its successors have been remarkably successful at both locating atomic sites and at assigning atomic types even for quite complicated structures - given an accurate estimate of the atomic composition. Even so, every Service Analyst will know that fully automatic determination of crystal structures is still a dream. The 'crystal-in ORTEP-out' black box may work for some structures, but examination of 500 structures completed by the service analyst in Oxford indicated that 30% of 'small' organic and 60% of organometallic structures need human intervention for their completion.

This leads us to ask 'What do humans know that programs don't, and what can humans do that programs cannot?'

The answer to the first question is that humans can develop a real understanding of chemistry and physics, so that they have a completely independent check on the plausibility of a proposed structure. In the event that something goes wrong this knowledge plus imagination enables them to propose alternative solutions.

The answer to the second question is that humans can learn from their own and other peoples experience. Current crystallographic programs can only do (if one is lucky) what their designer intended them to do. Some years ago, in the heyday of Artificial Intelligence, there seemed to be the prospect of programs improving their own reaction to problems, but so far this technology has made little impact in crystallography. If the resources being spent on Google were available to crystallographers, things might be very different.

For the moment we must base our confidence in automatically determined structures on the findings of programs such as PLATON, CHECKCIF and MOGUL. These may spot when things have gone wrong, but it will still take human imagination to put difficult cases right.

[1] (Rollett, J.S. 'Least Squares Procedures', in Crystallographic Computing, Ed Ahmed, 1970).