It is not about what the program *does* but about what *results* are expected.
Olex2 enables any scientist with an interest in single-crystal diffraction to perform all aspects of structure solution, refinement and publication tasks correctly and, in routine cases, without the need to refer to a trained crystallographer. This is achieved through a strong emphasis on workflow, combined with clear and indicative visual feedback of what is happening in any given task, on the way towards a publishable small-molecule structure. This makes Olex2 a very useful aid in teaching of small-molecule crystallography.
Olex2 is open source software and is available free of charge to academic users from http://www.olex2.org

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The Ambiguous Solutions from Different Automatic Structure Solution Programs.

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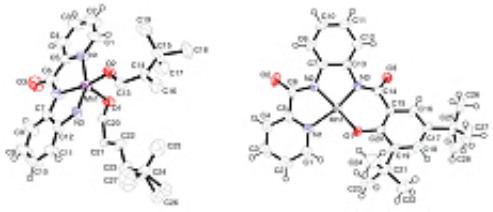
The manganese (III) complex with a diamide ligand has been synthesized by Lien-Hoa Tran. This complex was found to catalyze both epoxidation of (Z)- and (E)-stilbene with high conversion and the oxidation of benzyl alcohol to benzaldehyde. In this study we present the two different results of the different automatic structure solution programs.
First the structure was solved by direct methods using the SHELXS-97 [1] program. But the structure predicted from chemical and spectral analysis was not confirmed by X-ray analysis of the single crystal. Even though it had a satisfactory R(F) value of 0.0588 (*w*R(F) = 0.1153) and the minimum and maximum values for the residual density were -0.340 and 0.460 eÅ^{-3} respectively (Figure 1a).
Then SIR92 [2] was used in order to find the correct structure. The structure supported by chemical and spectral analysis was found (Figure 1b). At the final convergence limit the reliability indices are as follows: $R(F)$ = 0.0425, $wR(F)$ = 0.0772 and g.o.f. = 0.839. And the minimum and maximum values for the residual charge density were -0.222 and 0.227 eÅ^{-3} respectively.
In this study we see that the structure validation values such as R(F), *w*R(F), ρ_{max}, ρ_{min}, g.o.f, etc. are not satisfactory in order to define the correct crystal structure. It is interesting that both structures are “well behaved” but one of them is better.



(a) (b)

Figure 1. (a) Structure found by SHELXS-97 and (b) SIR92

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