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- A small indication of systematic error for \( U_{eq}' \) is observed only in one case, while in all the other cases this kind of error is quite negligible. In all cases the differences of the \( U_{eq}' \) from the two refinements are rather small.
- The \( R \) and \( wR \) (both for the \( R^2 \) refinement; \( wR^2 = \sum w(Fo - Fc)^2 / \sum w(Fo)^2 \) ) increase from 1.9 to 3.3 approximately linearly with the increasing of \( wR \) as a consequence of the fact that \( wR \) tends to become equal to \( wR^2 \) when the difference between \( F_o \) and \( F_c \) is small and increases with the increasing of this difference (i.e. with \( wR^2 \) or \( R^2 \)).
- The e.s.d.'s of the refined parameters from the \( R^2 \) refinement are lower than those from the \( F^2 \) refinement and this is not only an obvious consequence of the larger number of observations used in the first refinement, as the improvement tends to be more rapid when there is a large percentage of weak data and is also observed for the agreement between the chemically but not crystallographically equivalent bond lengths.
- The authors are grateful to Professor G.M. Sheldrick for his useful comments on the results of this analysis.

**PS-02.08.15 SIR92: A POWERFUL DIRECT METHODS PACKAGE**

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SIR92 is the powerful heir of SIR88 (M.C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna and D. Viterbo, J. Appl. Cryst., 1989, 22, 395-393) has shown to be a powerful tool to solve complex structures by Direct Methods. One-phase and two-phases semivariations and also are used to overcome difficulties arising from possible wrong estimations. Also SIR92 uses in an extensively way the Representation Theory. The main features are:
- new multisolution procedures (active use of negative triplets, negative quartets and psi-zero relationships);
- random starting set;
- automatic detection of not measured reflections and possibility to estimate them;
- new powerful figures of merit;
- automatic LSQ + Fourier procedure to obtain the correct and complete structure starting from E-map peaks;
- monitoring in real time of the completion of the structure on graphic display and possibility to interactively modify the model. Very difficult structures to solve by SIR88 (and other programs) are now solved as a routinary job by SIR92.