- A small indication of systematic error for U_{eq}'s is observed only in one case, while in all the other cases this kind of error is quite negligeable. In all cases the differences of the U_{eq}'s from the two refinements are rather small.
- The $R_{wU}=[\Sigma(w\Delta U)^2/T(wU_o)^2]^{1/2}$, $\Delta U=U_{ij}(obs.)-U_{ij}(calc.)$, index calculated on the basis of the rigid-body model (V. Schomaker & K.N. Trueblood, Acta Cryst. (1968). B24, 63-76) does not show great difference for the two refinements with some tendency to have a better agreement for the F^2 refinements.
- The ratio between the residual error indices wR_2/R_1 (both for the F^2 refinement; $wR_2=[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$, $R_1=\Sigma|F_o-F_c|/\Sigma F_o$) increases from 1.9 to 3.1 approximately linearly with the increasing of wR_2 as a consequence of the fact that wR_2 tends to become equal to $2R_1$ 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_1).
- The e.s.d.'s of the refined parameters from the F^2 refinement are lower than those from the F 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 most marked 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.

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PS-02.08.14 TRIPLET AND QUARTET RELATIONSHIPS AND THE POSITIVITY POSTULATE. By A. Altomare[*], C. Giacovazzo, A. Guagliardi, Dipartimento Geomineralogico, Universita' di Bari, 70124 Bari, Italy; D. Siliqi, Department of Inorganic Chemistry , University of Tirana, Tirana, Albania.

Positivity and atomicity are traditionally considered as basic conditions for direct methods. The origin of this belief traces back to the early theory of inequalities. Latter on it was perceived that positivity is not an essential ingredient of direct methods, however its role is not completely understood. No paper has so far been devoted to the description of the consequences on the phase relationships generated by the violation of the positivity condition and on its practical effects on direct phasing procedures. This is the first aim of this communication which analyzes triplet and quartet relationships in connection with the positivity postulate.

PS-02.08.15 SIR92: A POWERFUL DIRECT METHODS PACKAGE. By A. Altomare, G. Cascarano[*], C. Giacovazzo, A. Guagliardi, Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche, CNR, c/o Dipartimento Geomineralogico, Universita' di Bari, 70124 Bari, Italy; M. Camalli, Ist. di Strutturistica Chimica "G. Giacomello", CNR, Via Salaria Km 29,200, 00016 Monterotondo Stazione, Roma; M.C. Burla, G. Polidori, Dipartimento di Scienze della Terra, Universita', 06100 Perugia, Italy.

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, 22,389-393) has shown to be a powerful tool to solve complex structures by Direct Methods. One-phase and two-phases seminvariants, triplet and quartet invariants 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 refletions 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.