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Traditionally, crystallographic programs are run from a few standard data files for routine tasks, edited with the values for the current compound and run as batch jobs. For non-routine tasks the user is left searching the manual for elusive information.

An alternative modern strategy provides the user with a menu of procedures. This can be a useful facility for routine tasks, but offers the user little help with obscure or unusual problems.

In CRYSTALS we provide both of these input modes together with an interrogative interface through which the program enters into a dialogue with the user. This dialogue is driven by external 'scripts', and so can be tailored to suit novices (as a teaching aid), to simplify routine tasks, or as an aid for attacking unusual problems.

Since the user can write his own scripts, he can encode in them any special knowledge or experience he has. Since SCRIPTS can read data files, 'call' other SCRIPTS, and can even write new SCRIPTS themselves, the concept has the potential to be developed into an 'Expert System'.

At the meeting we will be showing, as an example, a script written to assist in the anisotropic refinement of large organo metallic compounds containing very many organic ligands and counter ions. Because each script is just a plain language ASCII data file, users can easiy modify them to handle local problems without risk of corrupting the CRYSTALS program itself.

The integration of a wide range of refinement, Fourier, geometry, graphical and analytical functions into a single package which can be used both interactively and in batch, which runs with identical functionality on anything between a PC386 and mainframes like the CONVEX makes CRYSTALS suitable for almost any environment or problem.

For users able to work interactively, there are integrated graphics which can be used both for the production of diagrams for publication, and as a powerful tool when dealing with large structures. The integration of Fourier map contouring with principal axis and TLS analysis of molecules is of great value for understanding disorder and thermal motion.

The ability to switch between the various user modes at will provides the flexibility needed for efficient structure analysis.

Enquiries about obtaining CRYSTALS should be addressed to David Watkin at the address above.

PS-02.08.12 THE ESTIMATION OF PHASE INVARIANTS FOR LARGE DIRECT METHODS STRUCTURE DETERMINATIONS. By D. A. Langs* and D.-Y. Guo, Department of Molecular Biophysics, Medical Foundation of Buffalo, Inc., 73 High Street, Buffalo, NY, U.S.A.

Simple tangent formula phase determination methods usually reach their limit of applicability when the complexity of a light atom structure exceeds 100 to 150 atoms. A new frequency-based triples phase invariant estimation procedure (Langs, Acta Cryst., **A49**, 1993, in press), employing traditional quadrupole relationships, has been shown to be successfully applicable to tangent formula structure determinations of greater than 300 atoms complexity. Efforts to extend the reliability of these frequency-based cosine invariant estimates by exploring higher-order relationships among phase invariants is in progress. Our experience using higher than 4th order Karle-Hauptman determinantal constructions has not been overly encouraging. We have however discovered one particularly interesting high order relationship involving 15 E-magnitudes that is most unusual in that it often embeds an unexpectedly high percentage of aberrant triples which have large A-values. We are currently exploring whether the frequency criterion or derived probability distribution can take advantage of these 15-magnitude constructs to forcefully disclose the identity of the embedded negative triples cosine invariants. If this can be achieved we strongly feel that this information will permit the solution of many more structures of greater than 300 atoms complexity by direct phasing methods.

Research support from NIH grant GM-46733 is gratefully acknowledged.

PS-02.08.13 COMPARISON OF F AND F^2 STANDARD REFINEMENTS OF SMALL MOLECULE CRYSTAL STRUCTURES. By S. Ianelli, M. Nardelli*, Istituto di Chimica Generale, Università di Parma, Centro di Studio CNR per la Strutturistica Diffrattometrica, Viale delle Scienze 78, I-43100 Parma, Italy.

It has been demonstrated that, in least-squares refinement of crystal structures, exclusion of weak (or "negative") intensities leads to a bias in the remaining experimental data towards too high F^2 values and thus to systematic errors in the refined parameters (F.L. Hirshfeld & D. Rabinovich, *Acta Cryst.* (1973). **A29**, 510-513; L. Arnberg, S. Hovmöller & S. Westman, *Acta Cryst.* (1979). **A35**, 497-499; P. Seiler, W.B. Schweizer & J.D. Dunitz, *Acta Cryst.* (1984). **B40**, 319-327). It seems that, omitting F's smaller than some predetermined size have some effect in the refinement that should be more important for scaling factors and temperature factors than for positional parameters. Moreover, carrying out two refinements with different weighting schemes might reveal the presence of significant but unsuspected defects in the model or systematic errors in the measurements (A.J.C. Wilson, *Acta Cryst.* (1973). **B29**, 1488-1480).
Taking the opportunity of checking the new born SHELXL-92 system for refinement of crystal structures (gamma-test stage) that is based on the use of F^2's, fifteen crystal structures of small organic and metal-organic molecules were refined, using data of standard quality, both on F (by using SHELX-76) and F^2. The results were compared using the half-normal probability plot technique (S.C. Abrahams & E.T. Keve, *Acta Cryst.* (1971). **A27**, 157-165) applied to all the interatomic distances less than 4.65 Å (W.H. De Camp, *Acta Cryst.* (1973). **A29**, 148-150) and to the U_{eq} values. The main results can be summarized as follows:
- The positional parameters obtained through these refinements are in general not significantly different, as only a limited number of long contacts have $\Delta/\sigma > 3$, which means that significant differences may be present only in some values of bonds and mainly torsion angles.
- No indication of systematic errors of some relevance is observed for positional parameters in the major number of cases. For these parameters in six cases the standard deviations are overestimated by factors ranging from 1.06 to 1.7, while in all the other cases the e.s.d.'s are underestimated by factors ranging from 1.07 to 2.25.

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- 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 $R_{wU}=[\Sigma(w\Delta U)^2/\mathrm{T}(wU_o)^2]^{1/2}$, $\Delta U=U_{ij}(\mathrm{obs.})-U_{ij}(\mathrm{calc.})$, 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.

The authors are grateful to Professor G.M. Sheldrick for his useful comments on the results of this analysis.

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.